09/734,625

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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	SEP 01	New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!
NEWS	4	OCT 28	KOREAPAT now available on STN
NEWS	5	NOV 30	PHAR reloaded with additional data
NEWS	6	DEC 01	LISA now available on STN
NEWS	7	DEC 09	12 databases to be removed from STN on December 31, 2004
NEWS	8	DEC 15	MEDLINE update schedule for December 2004
NEWS	9	DEC 17	ELCOM reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	10	DEC 17	COMPUAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	11	DEC 17	SOLIDSTATE reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	12	DEC 17	CERAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	13	DEC 17	THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
NEWS	14	DEC 30	EPFULL: New patent full text database to be available on STN
NEWS	15	DEC 30	CAPLUS - PATENT COVERAGE EXPANDED
NEWS	16	JAN 03	No connect-hour charges in EPFULL during January and February 2005
NEWS	17	JAN 26	CA/CAPLUS - Expanded patent coverage to include the Russian Agency for Patents and Trademarks (ROSPATENT)

NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:50:59 ON 06 FEB 2005

=> fil reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:51:10 ON 06 FEB 2005

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 4 FEB 2005 HIGHEST RN 825667-31-0
DICTIONARY FILE UPDATES: 4 FEB 2005 HIGHEST RN 825667-31-0

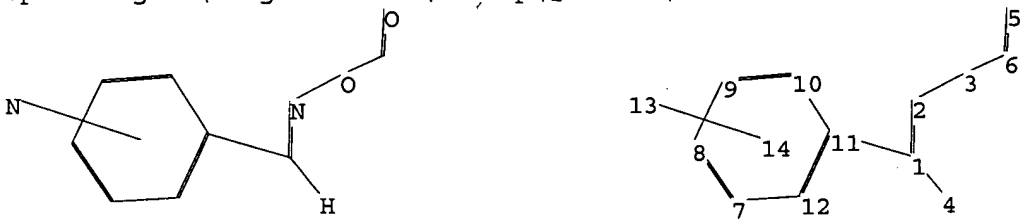
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\09734625.str

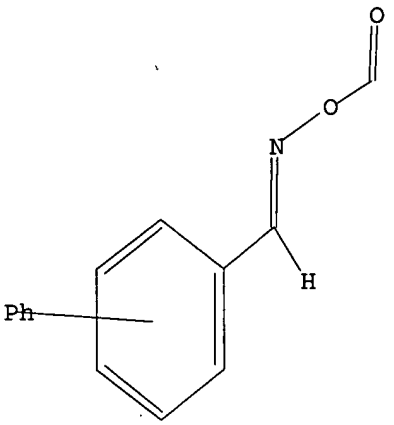


chain nodes :
1 2 3 4 5 6 13
ring nodes :
7 8 9 10 11 12
chain bonds :
1-2 1-4 1-11 2-3 3-6 5-6
ring bonds :
7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-2 2-3 3-6 5-6
exact bonds :
1-4 1-11
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS

L1 STRUCTURE UPLOADED

=> d query
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 ful
FULL SEARCH INITIATED 14:51:30 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 20775 TO ITERATE

100.0% PROCESSED 20775 ITERATIONS 10 ANSWERS
SEARCH TIME: 00.00.01

L2 10 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	161.33	161.54

FILE 'CAPLUS' ENTERED AT 14:51:33 ON 06 FEB 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 6 Feb 2005 VOL 142 ISS 7
FILE LAST UPDATED: 4 Feb 2005 (20050204/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s l2
L3              4 L2

=> d l3 1-4 abs ibib hitstr
```

L3 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

AB The invention relates to a photopolymn. initiator of oxime ester for a photoresist composition, wherein the oxime is derivative of Ar1-C=N-OR1(H) (R1 = cycloalkanoyl, benzoyl, alkenoyl; Ar1 = aryl, aroyl). The photopolymn. initiator provides the alkali-developable light-sensitive photoresist composition, which shows the improved storageability, of the high resolution and the good storageability.

ACCESSION NUMBER: 2001:752026 CAPLUS
DOCUMENT NUMBER: 135:280493
TITLE: Photopolymerization initiator of oxime ester for light-sensitive photoresist composition
INVENTOR(S): Kunimoto, Kazuhiko; Oka, Hidetaka; Ohwa, Masaki; Tanabe, Junichi; Kura, Hisatoshi; Birbaum, Jean Luc
PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.
SOURCE: Fr. Demande, 171 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2802528	A1	20010622	FR 2000-16306	20001214
TW 499411	B	20020821	TW 2000-89123924	20001110
NL 1016815	A1	20010618	NL 2000-1016815	20001206
NL 1016815	C2	20020514		
GB 2358017	A1	20010711	GB 2000-29793	20001207
GB 2358017	B2	20020313		
SE 2000004564	A	20020612	SE 2000-4564	20001211
SE 522774	C2	20040302		
US 2001012596	A1	20010809	US 2000-734625	20001212
JP 2001233842	A2	20010828	JP 2000-377671	20001212
IT 1319688	B1	20031023	IT 2000-MI2676	20001212
CA 2328376	AA	20010615	CA 2000-2328376	20001213
FI 2000002730	A	20010616	FI 2000-2730	20001213
DE 10061947	A1	20010621	DE 2000-10061947	20001213
ES 2177438	A1	20021201	ES 2000-2977	20001213
ES 2177438	B1	20041016		
DK 200001878	A5	20010616	DK 2000-1878	20001214
BE 1013872	A5	20021105	BE 2000-789	20001214
CN 1299812	A	20010620	CN 2000-135980	20001215
BR 2000006379	A	20010724	BR 2000-6379	20001215

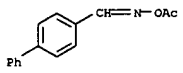
PRIORITY APPLN. INFO.:

EP 1999-811160	A	19991215
EP 2000-810629	A	20000717

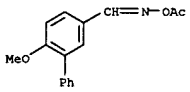
IT **362624-52-0P 362624-74-6P 362624-75-7P 362624-76-8P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(light-sensitive color filter composition containing oxime esters used in optical imaging devices)

RN 362624-52-0 CAPLUS
CN [1,1'-Biphenyl]-4-carboxaldehyde, O-acetyloxime (9CI) (CA INDEX NAME)

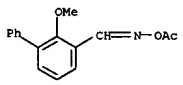
L3 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



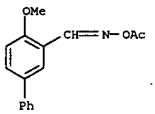
RN 362624-74-6 CAPLUS
CN [1,1'-Biphenyl]-3-carboxaldehyde, 6-methoxy-, O-acetyloxime (9CI) (CA INDEX NAME)



RN 362624-75-7 CAPLUS
CN [1,1'-Biphenyl]-3-carboxaldehyde, 2-methoxy-, O-acetyloxime (9CI) (CA INDEX NAME)



RN 362624-76-8 CAPLUS
CN [1,1'-Biphenyl]-3-carboxaldehyde, 4-methoxy-, O-acetyloxime (9CI) (CA INDEX NAME)



L3 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

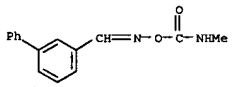
AB In dealing with the passive transport of organic contaminants from soils to plants (including crops), a partition-limited model is proposed in which (i) the maximum (equilibrium) concentration of a contaminant in any location in the plant is determined by partition equilibrium with its concentration in the soil interstitial water, which in turn is determined essentially by the concentration in the soil organic matter (SOM) and (ii) the extent of approach to partition equilibrium, as measured by the ratio of the contaminant concns. in plant water and soil interstitial water, αpt (≤ 1), depends on the transport rate of the contaminant in soil water into the plant and the volume of soil water solution that is required for the plant contaminant level to reach equilibrium with the external soil-water phase. Through reasonable ests. of plant organic-water compns. and of contaminant partition coeffs. with various plant components, the model accounts for calculated values of αpt in several published crop-contamination studies, including near-equilibrium values (i.e., αpt equivalent 1) for relatively water-soluble contaminants and lower values for much less soluble contaminants; the differences are attributed to the much higher partition coeffs. of the less soluble compds. between plant lipids and plant water, which necessitates much larger vols. of the plant water transport for achieving the equilibrium capacities. The model anal. indicates that for plants with high water contents the plant-water phase acts as the major reservoir for highly water-soluble contaminants. By contrast, the lipid in a plant, even at small amts., is usually the major reservoir for highly water-insol. contaminants.

ACCESSION NUMBER: 2001:149493 CAPLUS
DOCUMENT NUMBER: 134:321868
TITLE: A Partition-Limited Model for the Plant Uptake of Organic Contaminants from Soil and Water
AUTHOR(S): Chiou, Cary T.; Sheng, Guangyao; Manes, Milton
CORPORATE SOURCE: Denver Federal Center, U.S. Geological Survey, Denver, CO, 80225, USA
SOURCE: Environmental Science and Technology (2001), 35(7), 1437-1444
CODEN: ESTHAG; ISSN: 0013-936X
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **336784-32-8**, 3-Phenylbenzaldehyde O-methylcarbamoyl oxime
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(partition-limited model for plant uptake of organic contaminants from soil and water)

RN 336784-32-8 CAPLUS
CN [1,1'-Biphenyl]-3-carboxaldehyde, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)

L3 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

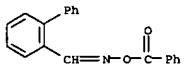
L3 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

AB Biphenyl-2-yl- and triarylvinyliminyls, generated by oxidation of the corresponding iminooxyacetic acids with persulfate and by the thermolysis of their tert-Bu peresters, underwent cyclization in high yield to give phenanthridines and quinolines, resp. E.g., o-PhC6H4CH:NOCH2CO2H and Ph2C:CPhCPh:NOCH2CO2H with persulfate gave 80% (by gas chromatog.) phenanthridine and 91% 2,3,4-triphenylquinoline, resp.

ACCESSION NUMBER: 1979:491472 CAPLUS
DOCUMENT NUMBER: 91:91472
TITLE: Iminyls. Part 2. Intramolecular aromatic substitution by iminyls. A new route to phenanthridines and quinolines
AUTHOR(S): Forrester, Alexander R.; Gill, Melvyn; Sadd, John S.; Thomson, Ronald H.
CORPORATE SOURCE: Chem. Dep., Univ. Aberdeen, Aberdeen, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1979), (3), 612-15
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English

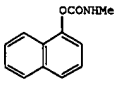
IT **71103-62-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 71103-62-3 CAPLUS
CN [1,1'-Biphenyl]-2-carboxaldehyde, O-benzoyloxime (9CI) (CA INDEX NAME)



L3 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

GI



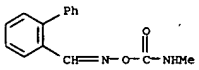
I

AB The anticholinesterase activity of Sevin (I) [63-25-2] and 25 biphenyl, furylbenzene, fluorene, and tetraline derivs. was determined by IR and NMR measurements of inhibition of acetylcholine hydrolysis by pseudocholinesterase. The media used were H2O-dioxane for the NMR and D2O-dioxane for the IR measurement. The method may be used for screening of potential insecticides. The relations between structure and anticholinesterase and insecticidal activities are discussed.

ACCESSION NUMBER: 1977:38457 CAPLUS
DOCUMENT NUMBER: 86:38457
TITLE: Spectroscopic measurement of cholinesterase activity. III. NMR and IR spectroscopic determination of anticholinesterase activity of carbamate insecticides
AUTHOR(S): Ronzani, Nello; Guillochon, Didier; Lange, Catherine; Basselier, Jean J.
CORPORATE SOURCE: Lab. Chim. Org. Struct., Paris, Fr.
SOURCE: European Journal of Medicinal Chemistry (1976), 11(4), 310-15
CODEN: EJMCA5; ISSN: 0223-5234
DOCUMENT TYPE: Journal
LANGUAGE: French

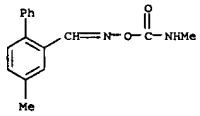
IT **61518-10-3 61518-11-4 61518-12-5 61518-13-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(anticholinesterase activity of, determination of)

RN 61518-10-3 CAPLUS
CN [1,1'-Biphenyl]-2-carboxaldehyde, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)

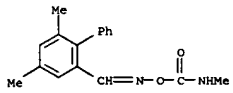


RN 61518-11-4 CAPLUS
CN [1,1'-Biphenyl]-2-carboxaldehyde, 4-methyl-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)

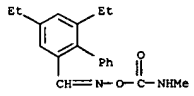
L3 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 61518-12-5 CAPLUS
CN [1,1'-Biphenyl]-2-carboxaldehyde, 4,6-dimethyl-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



RN 61518-13-6 CAPLUS
CN [1,1'-Biphenyl]-2-carboxaldehyde, 4,6-diethyl-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



=> fil reg
COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 22.46 | 184.00

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION
CA SUBSCRIBER PRICE | -2.92 | -2.92

FILE 'REGISTRY' ENTERED AT 14:55:05 ON 06 FEB 2005
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 4 FEB 2005 HIGHEST RN 825667-31-0
DICTIONARY FILE UPDATES: 4 FEB 2005 HIGHEST RN 825667-31-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

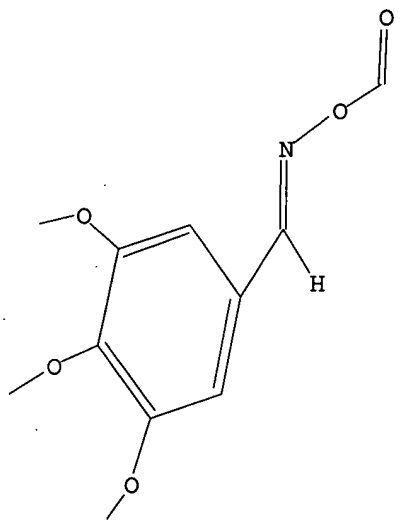
=>
Uploading C:\Program Files\Stnexp\Queries\09734625.str

chain nodes :
1 2 3 4 5 6 13
ring nodes :
7 8 9 10 11 12
chain bonds :
1-2 1-4 1-11 2-3 3-6 5-6
ring bonds :
7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-2 2-3 3-6 5-6
exact bonds :
1-4 1-11
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS

L4 STRUCTURE UPLOADED

=> d query
L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l4
SAMPLE SEARCH INITIATED 14:56:31 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 11 TO ITERATE

100.0% PROCESSED 11 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 22 TO 418
PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> s l4 full
FULL SEARCH INITIATED 14:56:36 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 212 TO ITERATE

100.0% PROCESSED 212 ITERATIONS 57 ANSWERS
SEARCH TIME: 00.00.01

L6 57 SEA SSS FUL L4

```
=> fil caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                    162.19     346.19

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                      0.00      -2.92

FILE 'CAPLUS' ENTERED AT 14:56:41 ON 06 FEB 2005
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FILE COVERS 1907 - 6 Feb 2005  VOL 142 ISS 7
FILE LAST UPDATED: 4 Feb 2005  (20050204/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l6
L7            2 L6

=> d l7 1-2 abs ibib hitstr
```

L7 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

AB The invention relates to a photopolymn. initiator of oxime ester for a photoresist composition, wherein the oxime is derivative of Ar1-C=N-OR1(H) (R1 = cycloalkanoyl, benzoyl, alkenoyl; Ar1 = aryl, aroyl). The photopolymn. initiator provides the alkali-developable light-sensitive photoresist composition, which shows the improved storageability, of the high resolution and the good storageability.

ACCESSION NUMBER: 2001:752026 CAPLUS
DOCUMENT NUMBER: 135:280493
TITLE: Photopolymerization initiator of oxime ester for light-sensitive photoresist composition
INVENTOR(S): Kunimoto, Kazuhiko; Oka, Hidetaka; Ohwa, Masaki; Tanabe, Junichi; Kura, Hisatoshi; Birbaum, Jean Luc
PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.
SOURCE: Fr. Demande, 171 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

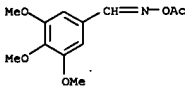
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2802528	A1	20010622	FR 2000-16306	20001214
TW 499411	B	20020821	TW 2000-89123924	20001110
NL 1016815	A1	20010618	NL 2000-1016815	20001206
NL 1016815	C2	20020514		
GB 2358017	A1	20010711	GB 2000-29793	20001207
GB 2358017	B2	20020313		
SE 2000004564	A	20020612	SE 2000-4564	20001211
SE 522774	C2	20040302		
US 2001012596	A1	20010809	US 2000-734625	20001212
JP 2001233842	A2	20010828	JP 2000-377671	20001212
IT 1319688	B1	20031023	IT 2000-MI2676	20001212
CA 2328376	AA	20010615	CA 2000-2328376	20001213
FI 2000002730	A	20010616	FI 2000-2730	20001213
DE 10061947	A1	20010621	DE 2000-10061947	20001213
ES 2177438	A1	20021201	ES 2000-2977	20001213
ES 2177438	B1	20041016		
DK 200001878	A5	20010616	DK 2000-1878	20001214
BE 1013872	A5	20021105	BE 2000-789	20001214
CN 1299812	A	20010620	CN 2000-135980	20001215
BR 2000006379	A	20010724	BR 2000-6379	20001215

PRIORITY APPLN. INFO.:
EP 1999-811160 A 19991215
EP 2000-810629 A 20000717

IT **333438-68-9P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(light-sensitive color filter composition containing oxime esters used in optical imaging devices)

RN 333438-68-9 CAPLUS
CN Benzaldehyde, 3,4,5-trimethoxy-, O-acetyloxime (9CI) (CA INDEX NAME)

L7 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



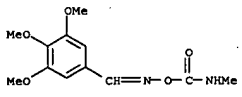
L7 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

AB Carbaryl was applied topically, singly, and in combination with several series of adjuvants to the housefly to determine the role of the dioxole ring of methylenedioxyphenyl compds. in synergizing the carbamate insecticides. When the methylenedioxy moiety was replaced with methoxyl or methoxyl and hydroxyl groups, synergistic activity was greatly reduced or lost. Several 1,3-benzodioxans also failed to act as synergists. The integrity of the 1,2-methylenedioxy structure is essential for maximum potentiation of housefly toxicity of the carbamates, paralleling the case for pyrethrins synergism.

ACCESSION NUMBER: 1965:25221 CAPLUS
DOCUMENT NUMBER: 62:25221
ORIGINAL REFERENCE NO.: 62:4549f-g
TITLE: Influence of the methylenedioxyphenyl structure in synergism of a carbamate insecticide for house flies
AUTHOR(S): Moorefield, Herbert H.; Weiden, Mathias H. J.
CORPORATE SOURCE: Union Carbide Agr. Res. Sta., Clayton, NC
SOURCE: Contributions from Boyce Thompson Institute (1964), 22(8), 425-33
CODEN: CBTIAE; ISSN: 0006-8543
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **2815-72-7**, Benzaldehyde, 3,4,5-trimethoxy-, O-(methylcarbamoyl)oxime
(as synergist for carbaryl, in housefly control)

RN 2815-72-7 CAPLUS
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(methylcarbamoyl)oxime (7CI, 8CI) (CA INDEX NAME)



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                                                           ENTRY    SESSION
FULL ESTIMATED COST                                        10.78     356.97

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)              SINCE FILE      TOTAL
                                                           ENTRY    SESSION
CA SUBSCRIBER PRICE                                        -1.46      -4.38

FILE 'REGISTRY' ENTERED AT 14:57:52 ON 06 FEB 2005
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STRUCTURE FILE UPDATES:    4 FEB 2005  HIGHEST RN 825667-31-0
DICTIONARY FILE UPDATES:   4 FEB 2005  HIGHEST RN 825667-31-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         0.43     357.40

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)              SINCE FILE      TOTAL
                                                           ENTRY    SESSION
CA SUBSCRIBER PRICE                                         0.00      -4.38

FILE 'REGISTRY' ENTERED AT 14:58:11 ON 06 FEB 2005
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STRUCTURE FILE UPDATES:    4 FEB 2005  HIGHEST RN 825667-31-0
DICTIONARY FILE UPDATES:   4 FEB 2005  HIGHEST RN 825667-31-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.
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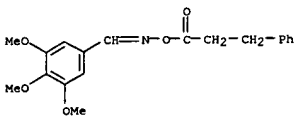
Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

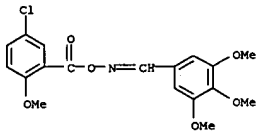
=> d l6 1-57

L6 ANSWER 1 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409338-28-9 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(1-oxo-3-phenylpropyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H21 N O5
SR Chemical Library
LC STN Files: CHEMCATS



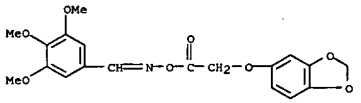
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 2 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409337-99-1 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(5-chloro-2-methoxybenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H18 Cl N O6
SR Chemical Library
LC STN Files: CHEMCATS



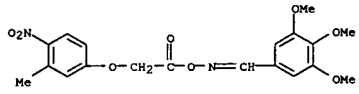
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 3 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409337-93-5 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(1,3-benzodioxol-5-yloxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H19 N O8
SR Chemical Library
LC STN Files: CHEMCATS



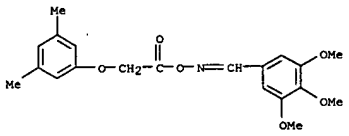
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 4 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409337-84-4 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(3-methyl-4-nitrophenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H20 N2 O8
SR Chemical Library
LC STN Files: CHEMCATS



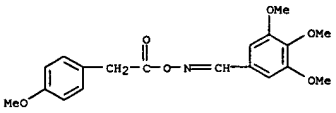
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 5 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409337-43-5 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(3,5-dimethylphenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H23 N O6
SR Chemical Library
LC STN Files: CHEMCATS



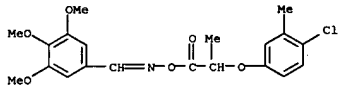
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 6 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409337-21-9 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(4-methoxyphenyl)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H21 N O6
SR Chemical Library
LC STN Files: CHEMCATS



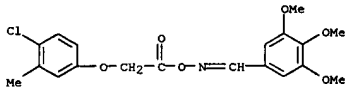
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 7 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409312-01-2 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[2-(4-chloro-3-methylphenoxy)-1-oxopropyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H22 Cl N O6
SR Chemical Library
LC STN Files: CHEMCATS



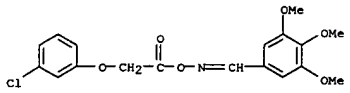
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 8 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409311-99-5 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(4-chloro-3-methylphenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H20 Cl N O6
SR Chemical Library
LC STN Files: CHEMCATS



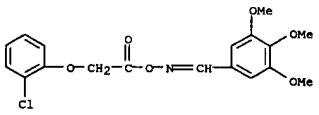
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 9 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409311-83-7 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(3-chlorophenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H18 Cl N O6
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 10 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409310-57-2 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(2-chlorophenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H18 Cl N O6
SR Chemical Library
LC STN Files: CHEMCATS



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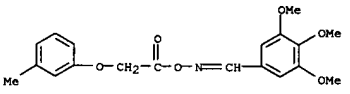
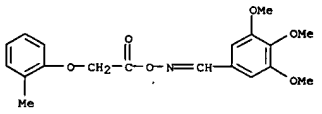
L6 ANSWER 11 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409310-51-6 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(3-methylphenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H21 N O6
SR Chemical Library
LC STN Files: CHEMCATS



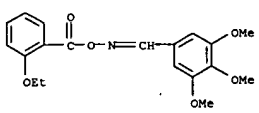
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 12 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409309-67-7 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(2-methylphenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H21 N O6
SR Chemical Library
LC STN Files: CHEMCATS



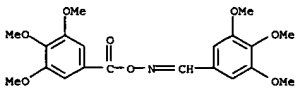
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 13 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409308-82-3 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-ethoxybenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H21 N O6
SR Chemical Library
LC STN Files: CHEMCATS



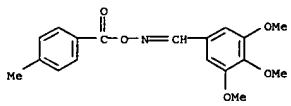
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 14 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409308-34-5 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(3,4,5-trimethoxybenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H23 N O8
SR Chemical Library
LC STN Files: CHEMCATS



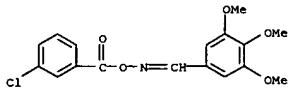
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 15 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409307-85-3 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(4-methylbenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H19 N O5
SR Chemical Library
LC STN Files: CHEMCATS



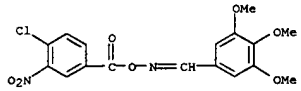
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 16 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409125-17-3 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(3-chlorobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H16 Cl N O5
SR Chemical Library
LC STN Files: CHEMCATS



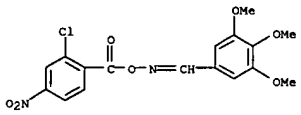
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 17 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409124-54-5 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(4-chloro-3-nitrobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H15 Cl N2 O7
SR Chemical Library
LC STN Files: CHEMCATS



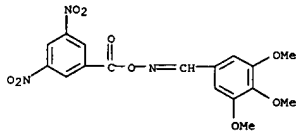
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 18 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409124-36-3 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-chloro-4-nitrobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H15 Cl N2 O7
SR Chemical Library
LC STN Files: CHEMCATS



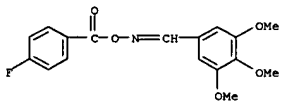
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 19 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409123-19-9 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(3,5-dinitrobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H15 N3 O9
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 20 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409122-57-2 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(4-fluorobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H16 F N O5
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 21 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409122-03-8 REGISTRY
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FS 3D CONCORD
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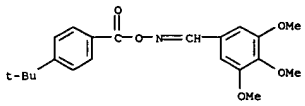
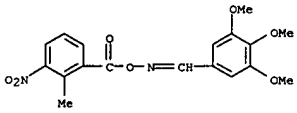
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 22 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409121-98-8 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-methyl-3-nitrobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H18 N2 O7
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 23 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409121-91-1 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-benzoyloxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H17 N O5
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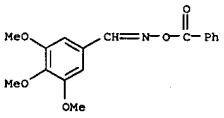
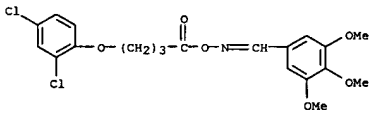
LC STN Files: CHEMCATS



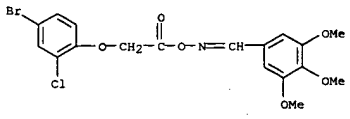
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 24 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409121-41-1 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[4-(2,4-dichlorophenoxy)-1-oxobutyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H21 Cl2 N O6
SR Chemical Library
LC STN Files: CHEMCATS



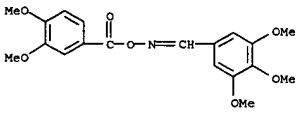
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 25 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409120-61-2 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(4-bromo-2-chlorophenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H17 Br Cl N O6
SR Chemical Library
LC STN Files: CHEMCATS



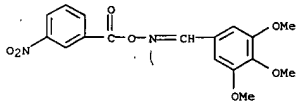
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 26 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409119-87-5 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(3,4-dimethoxybenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H21 N O7
SR Chemical Library
LC STN Files: CHEMCATS



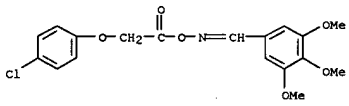
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 27 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409119-23-9 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(3-nitrobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H16 N2 O7
SR Chemical Library
LC STN Files: CHEMCATS



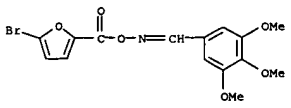
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 28 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409119-16-0 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(4-chlorophenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H18 Cl N O6
SR Chemical Library
LC STN Files: CHEMCATS



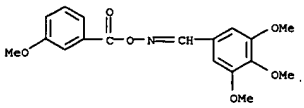
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 29 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409119-14-8 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(5-bromo-2-furanyl)carbonyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H14 Br N O6
SR Chemical Library
LC STN Files: CHEMCATS



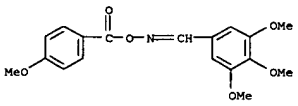
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 30 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409118-77-0 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(3-methoxybenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H19 N O6
SR Chemical Library
LC STN Files: CHEMCATS



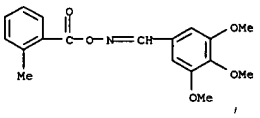
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 31 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409118-69-0 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(4-methoxybenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H19 N O6
SR Chemical Library
LC STN Files: CHEMCATS



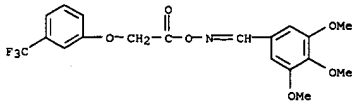
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 32 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409118-51-0 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-methylbenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H19 N O5
SR Chemical Library
LC STN Files: CHEMCATS



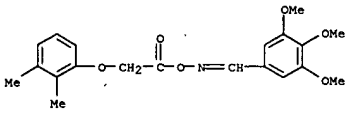
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 33 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409118-25-8 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[[3-(trifluoromethyl)phenoxy]acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H18 F3 N O6
SR Chemical Library
LC STN Files: CHEMCATS



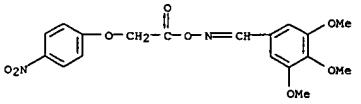
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 34 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409118-12-3 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(2,3-dimethylphenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H23 N O6
SR Chemical Library
LC STN Files: CHEMCATS



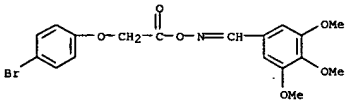
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 35 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409117-91-5 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(4-nitrophenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H18 N2 O8
SR Chemical Library
LC STN Files: CHEMCATS



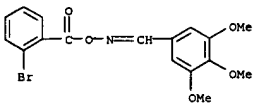
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 36 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409117-26-6 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(4-bromophenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H18 Br N O6
SR Chemical Library
LC STN Files: CHEMCATS



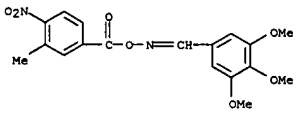
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 37 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409116-32-1 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-bromobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H16 Br N O5
SR Chemical Library
LC STN Files: CHEMCATS



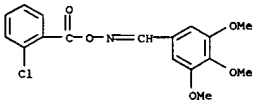
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 38 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409115-93-1 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(3-methyl-4-nitrobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H18 N2 O7
SR Chemical Library
LC STN Files: CHEMCATS



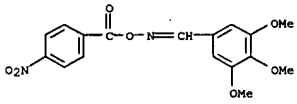
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 39 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409115-90-8 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-chlorobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H16 Cl N O5
SR Chemical Library
LC STN Files: CHEMCATS



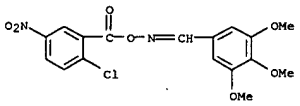
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 40 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409115-64-6 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(4-nitrobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H16 N2 O7
SR Chemical Library
LC STN Files: CHEMCATS



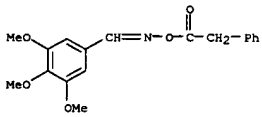
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 41 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409115-37-3 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-chloro-5-nitrobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H15 Cl N2 O7
SR Chemical Library
LC STN Files: CHEMCATS



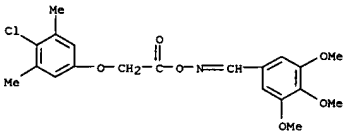
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 42 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409103-86-2 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(phenylacetyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H19 N O5
SR Chemical Library
LC STN Files: CHEMCATS



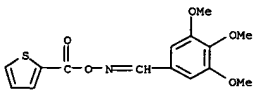
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 43 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409103-02-2 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(4-chloro-3,5-dimethylphenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H22 Cl N O6
SR Chemical Library
LC STN Files: CHEMCATS



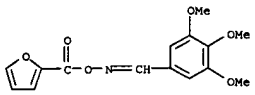
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 44 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409101-98-0 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-thienylcarbonyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H15 N O5 S
SR Chemical Library
LC STN Files: CHEMCATS



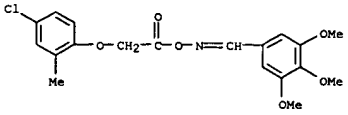
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 45 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409101-91-3 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-furanylcarbonyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H15 N O6
SR Chemical Library
LC STN Files: CHEMCATS



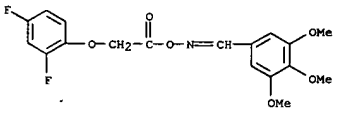
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 46 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409101-71-9 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(4-chloro-2-methylphenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H20 Cl N O6
SR Chemical Library
LC STN Files: CHEMCATS



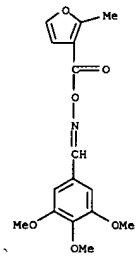
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 47 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409101-45-7 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(2,4-difluorophenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H17 F2 N O6
SR Chemical Library
LC STN Files: CHEMCATS



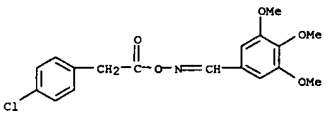
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 48 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409101-11-7 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(2-methyl-3-furanyl)carbonyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H17 N O6
SR Chemical Library
LC STN Files: CHEMCATS



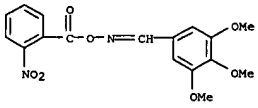
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 49 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409100-85-2 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(4-chlorophenyl)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H18 Cl N O5
SR Chemical Library
LC STN Files: CHEMCATS



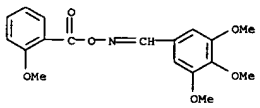
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 50 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409100-56-7 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-nitrobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H16 N2 O7
SR Chemical Library
LC STN Files: CHEMCATS



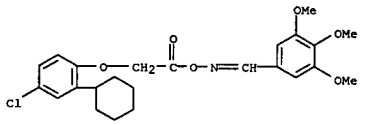
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 51 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409099-89-4 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-methoxybenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H19 N O6
SR Chemical Library
LC STN Files: CHEMCATS



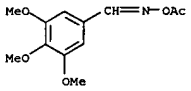
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 52 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409099-69-0 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(4-chloro-2-cyclohexylphenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C24 H28 Cl N O6
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

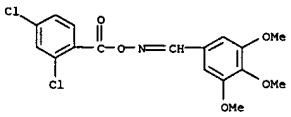
L6 ANSWER 53 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 333438-68-9 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-acetyloxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H15 N O5
SR Chemical Library
LC STN Files: CA, CAPLUS, CHEMCATS, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

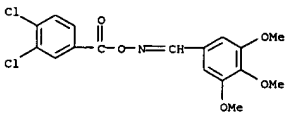
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 54 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 284679-88-5 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2,4-dichlorobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H15 Cl2 N O5
SR CAS Client Services
LC STN Files: CHEMCATS



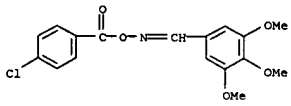
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 55 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 284679-87-4 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(3,4-dichlorobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H15 Cl2 N O5
SR CAS Client Services
LC STN Files: CHEMCATS



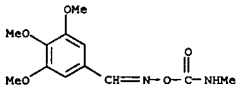
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 56 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 284679-86-3 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(4-chlorobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H16 Cl N O5
SR CAS Client Services
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 57 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 2815-72-7 REGISTRY
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(methylcarbamoyl)oxime (7CI, 8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H16 N2 O5
LC STN Files: CA, CAOLD, CAPLUS, TOXCENTER
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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=>  fil caplus
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                      106.17     463.57

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)            SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                        0.00      -4.38

FILE 'CAPLUS' ENTERED AT 14:59:41 ON 06 FEB 2005
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FILE COVERS 1907 - 6 Feb 2005  VOL 142 ISS 7
FILE LAST UPDATED: 4 Feb 2005  (20050204/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s 409100-56-7/rn
             0 409100-56-7
             0 409100-56-7D
L8           0 409100-56-7/RN
                 (409100-56-7 (NOTL) 409100-56-7D )

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COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                        4.23     467.80

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)            SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                        0.00      -4.38

FILE 'REGISTRY' ENTERED AT 15:00:14 ON 06 FEB 2005
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:    4 FEB 2005  HIGHEST RN 825667-31-0
DICTIONARY FILE UPDATES:   4 FEB 2005  HIGHEST RN 825667-31-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004
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Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

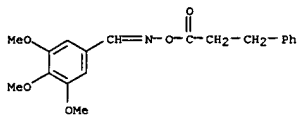
Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d l6 1-57 all

L6 ANSWER 1 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409338-28-9 REGISTRY
ED Entered STN: 01 May 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(1-oxo-3-phenylpropyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H21 N O5
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	875	pH 1	(1) ACD
Bioconc. Factor (BCF)	875	pH 4	(1) ACD
Bioconc. Factor (BCF)	875	pH 7	(1) ACD
Bioconc. Factor (BCF)	875	pH 8	(1) ACD
Bioconc. Factor (BCF)	875	pH 10	(1) ACD
Boiling Point (BP)	479.5+/-50.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	74.38+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	191.8+/-44.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	8		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	4442	pH 1	(1) ACD
Koc (KOC)	4442	pH 4	(1) ACD
Koc (KOC)	4442	pH 7	(1) ACD
Koc (KOC)	4442	pH 8	(1) ACD
Koc (KOC)	4442	pH 10	(1) ACD
logD (LOGD)	4.17	pH 1	(1) ACD
logD (LOGD)	4.17	pH 4	(1) ACD
logD (LOGD)	4.17	pH 7	(1) ACD
logD (LOGD)	4.17	pH 8	(1) ACD
logD (LOGD)	4.17	pH 10	(1) ACD
logP (LOGP)	4.174+/-0.586		(1) ACD

L6 ANSWER 1 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	343.37		(1) ACD
Vapor Pressure (VP)	2.35E-09 Torr	25.0 deg C	(1) ACD

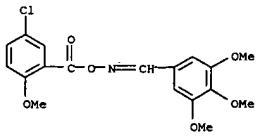
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 2 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409337-99-1 REGISTRY
ED Entered STN: 01 May 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(5-chloro-2-methoxybenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H18 Cl N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1194	pH 1	(1) ACD
Bioconc. Factor (BCF)	1194	pH 4	(1) ACD
Bioconc. Factor (BCF)	1194	pH 7	(1) ACD
Bioconc. Factor (BCF)	1194	pH 8	(1) ACD
Bioconc. Factor (BCF)	1194	pH 10	(1) ACD
Boiling Point (BP)	521.6+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	79.49+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	269.3+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	5548	pH 1	(1) ACD
Koc (KOC)	5548	pH 4	(1) ACD
Koc (KOC)	5548	pH 7	(1) ACD
Koc (KOC)	5548	pH 8	(1) ACD
Koc (KOC)	5548	pH 10	(1) ACD
logD (LOGD)	4.35	pH 1	(1) ACD
logD (LOGD)	4.35	pH 4	(1) ACD
logD (LOGD)	4.35	pH 7	(1) ACD
logD (LOGD)	4.35	pH 8	(1) ACD
logD (LOGD)	4.35	pH 10	(1) ACD

L6 ANSWER 2 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

logP (LOGP)	4.351+/-0.601		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	379.79		(1) ACD
Vapor Pressure (VP)	5.58E-11 Torr	25.0 deg C	(1) ACD

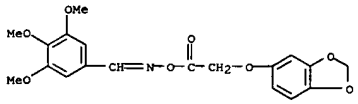
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 3 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409337-93-5 REGISTRY
ED Entered STN: 01 May 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(1,3-benzodioxol-5-yloxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H19 N O8
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1
C3O2-C6	OCOC2-C6	5-6	C7O2	333.584.8	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	250	pH 1	(1) ACD
Bioconc. Factor (BCF)	250	pH 4	(1) ACD
Bioconc. Factor (BCF)	250	pH 7	(1) ACD
Bioconc. Factor (BCF)	250	pH 8	(1) ACD
Bioconc. Factor (BCF)	250	pH 10	(1) ACD
Boiling Point (BP)	528.3+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	80.31+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	218.7+/-49.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	8		(1) ACD
H acceptors (HAC)	9		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	1814	pH 1	(1) ACD
Koc (KOC)	1814	pH 4	(1) ACD
Koc (KOC)	1814	pH 7	(1) ACD
Koc (KOC)	1814	pH 8	(1) ACD
Koc (KOC)	1814	pH 10	(1) ACD
logD (LOGD)	3.46	pH 1	(1) ACD
logD (LOGD)	3.46	pH 4	(1) ACD
logD (LOGD)	3.46	pH 7	(1) ACD
logD (LOGD)	3.46	pH 8	(1) ACD
logD (LOGD)	3.46	pH 10	(1) ACD
logP (LOGP)	3.459+/-0.626		(1) ACD

L6 ANSWER 3 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	389.36		(1) ACD
Vapor Pressure (VP)	2.99E-11 Torr	25.0 deg C	(1) ACD

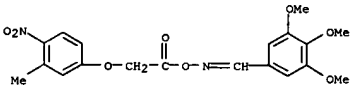
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 4 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409337-84-4 REGISTRY
ED Entered STN: 01 May 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(3-methyl-4-nitrophenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H20 N2 O8
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	596	pH 1	(1) ACD
Bioconc. Factor (BCF)	596	pH 4	(1) ACD
Bioconc. Factor (BCF)	596	pH 7	(1) ACD
Bioconc. Factor (BCF)	596	pH 8	(1) ACD
Bioconc. Factor (BCF)	596	pH 10	(1) ACD
Boiling Point (BP)	570.9+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	85.61+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	299.1+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	9		(1) ACD
H acceptors (HAC)	10		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	3375	pH 1	(1) ACD
Koc (KOC)	3375	pH 4	(1) ACD
Koc (KOC)	3375	pH 7	(1) ACD
Koc (KOC)	3375	pH 8	(1) ACD
Koc (KOC)	3375	pH 10	(1) ACD
logD (LOGD)	3.95	pH 1	(1) ACD
logD (LOGD)	3.95	pH 4	(1) ACD
logD (LOGD)	3.95	pH 7	(1) ACD
logD (LOGD)	3.95	pH 8	(1) ACD
logD (LOGD)	3.95	pH 10	(1) ACD
logP (LOGP)	3.955+/-0.610		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD

L6 ANSWER 4 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	404.37		(1) ACD
Vapor Pressure (VP)	4.82E-13 Torr	25.0 deg C	(1) ACD

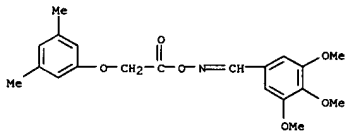
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 5 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409337-43-5 REGISTRY
ED Entered STN: 01 May 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(3,5-dimethylphenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H23 N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1599	pH 1	(1) ACD
Bioconc. Factor (BCF)	1599	pH 4	(1) ACD
Bioconc. Factor (BCF)	1599	pH 7	(1) ACD
Bioconc. Factor (BCF)	1599	pH 8	(1) ACD
Bioconc. Factor (BCF)	1599	pH 10	(1) ACD
Boiling Point (BP)	515.9+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	78.78+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	202.9+/-49.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	8		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	6839	pH 1	(1) ACD
Koc (KOC)	6839	pH 4	(1) ACD
Koc (KOC)	6839	pH 7	(1) ACD
Koc (KOC)	6839	pH 8	(1) ACD
Koc (KOC)	6839	pH 10	(1) ACD
logD (LOGD)	4.52	pH 1	(1) ACD
logD (LOGD)	4.52	pH 4	(1) ACD
logD (LOGD)	4.52	pH 7	(1) ACD
logD (LOGD)	4.52	pH 8	(1) ACD
logD (LOGD)	4.52	pH 10	(1) ACD

L6 ANSWER 5 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

logP (LOGP)	4.518+/-0.604		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	373.40		(1) ACD
Vapor Pressure (VP)	9.46E-11 Torr	25.0 deg C	(1) ACD

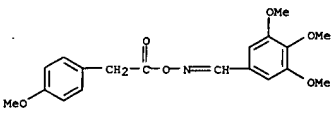
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 6 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409337-21-9 REGISTRY
ED Entered STN: 01 May 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(4-methoxyphenyl)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H21 N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	365	pH 1	(1) ACD
Bioconc. Factor (BCF)	365	pH 4	(1) ACD
Bioconc. Factor (BCF)	365	pH 7	(1) ACD
Bioconc. Factor (BCF)	365	pH 8	(1) ACD
Bioconc. Factor (BCF)	365	pH 10	(1) ACD
Boiling Point (BP)	499.1+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	76.74+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	200.8+/-46.7 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	8		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	2373	pH 1	(1) ACD
Koc (KOC)	2373	pH 4	(1) ACD
Koc (KOC)	2373	pH 7	(1) ACD
Koc (KOC)	2373	pH 8	(1) ACD
Koc (KOC)	2373	pH 10	(1) ACD
logD (LOGD)	3.67	pH 1	(1) ACD
logD (LOGD)	3.67	pH 4	(1) ACD
logD (LOGD)	3.67	pH 7	(1) ACD
logD (LOGD)	3.67	pH 8	(1) ACD
logD (LOGD)	3.67	pH 10	(1) ACD
logP (LOGP)	3.673+/-0.596		(1) ACD

L6 ANSWER 6 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	359.37		(1) ACD
Vapor Pressure (VP)	4.28E-10 Torr	25.0 deg C	(1) ACD

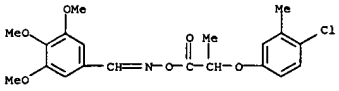
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 7 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409312-01-2 REGISTRY
ED Entered STN: 01 May 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[2-(4-chloro-3-methylphenoxy)-1-oxopropyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H22 Cl N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	4365	pH 1	(1) ACD
Bioconc. Factor (BCF)	4365	pH 4	(1) ACD
Bioconc. Factor (BCF)	4365	pH 7	(1) ACD
Bioconc. Factor (BCF)	4365	pH 8	(1) ACD
Bioconc. Factor (BCF)	4365	pH 10	(1) ACD
Boiling Point (BP)	529.8+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	80.49+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	274.2+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	8		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	14030	pH 1	(1) ACD
Koc (KOC)	14030	pH 4	(1) ACD
Koc (KOC)	14030	pH 7	(1) ACD
Koc (KOC)	14030	pH 8	(1) ACD
Koc (KOC)	14030	pH 10	(1) ACD
logD (LOGD)	5.09	pH 1	(1) ACD
logD (LOGD)	5.09	pH 4	(1) ACD
logD (LOGD)	5.09	pH 7	(1) ACD
logD (LOGD)	5.09	pH 8	(1) ACD
logD (LOGD)	5.09	pH 10	(1) ACD
logP (LOGP)	5.092+/-0.610		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD

L6 ANSWER 7 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	407.84		(1) ACD
Vapor Pressure (VP)	2.61E-11 Torr	25.0 deg C	(1) ACD

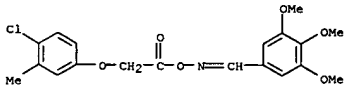
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 8 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409311-99-5 REGISTRY
ED Entered STN: 01 May 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(4-chloro-3-methylphenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H20 Cl N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	2376	pH 1	(1) ACD
Bioconc. Factor (BCF)	2376	pH 4	(1) ACD
Bioconc. Factor (BCF)	2376	pH 7	(1) ACD
Bioconc. Factor (BCF)	2376	pH 8	(1) ACD
Bioconc. Factor (BCF)	2376	pH 10	(1) ACD
Boiling Point (BP)	524.8+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	79.88+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	271.2+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	8		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	9080	pH 1	(1) ACD
Koc (KOC)	9080	pH 4	(1) ACD
Koc (KOC)	9080	pH 7	(1) ACD
Koc (KOC)	9080	pH 8	(1) ACD
Koc (KOC)	9080	pH 10	(1) ACD
logD (LOGD)	4.74	pH 1	(1) ACD
logD (LOGD)	4.74	pH 4	(1) ACD
logD (LOGD)	4.74	pH 7	(1) ACD
logD (LOGD)	4.74	pH 8	(1) ACD
logD (LOGD)	4.74	pH 10	(1) ACD
logP (LOGP)	4.745+/-0.609		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

L6 ANSWER 8 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	393.82		(1) ACD
Vapor Pressure (VP)	4.14E-11 Torr	25.0 deg C	(1) ACD

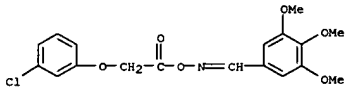
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 9 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409311-83-7 REGISTRY
ED Entered STN: 01 May 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(3-chlorophenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H18 Cl N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1359	pH 1	(1) ACD
Bioconc. Factor (BCF)	1359	pH 4	(1) ACD
Bioconc. Factor (BCF)	1359	pH 7	(1) ACD
Bioconc. Factor (BCF)	1359	pH 8	(1) ACD
Bioconc. Factor (BCF)	1359	pH 10	(1) ACD
Boiling Point (BP)	509.4+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	78.00+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	261.9+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	8		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	6086	pH 1	(1) ACD
Koc (KOC)	6086	pH 4	(1) ACD
Koc (KOC)	6086	pH 7	(1) ACD
Koc (KOC)	6086	pH 8	(1) ACD
Koc (KOC)	6086	pH 10	(1) ACD
logD (LOGD)	4.43	pH 1	(1) ACD
logD (LOGD)	4.43	pH 4	(1) ACD
logD (LOGD)	4.43	pH 7	(1) ACD
logD (LOGD)	4.43	pH 8	(1) ACD
logD (LOGD)	4.43	pH 10	(1) ACD
logP (LOGP)	4.425+/-0.608		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD

L6 ANSWER 9 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	379.79		(1) ACD
Vapor Pressure (VP)	1.70E-10 Torr	25.0 deg C	(1) ACD

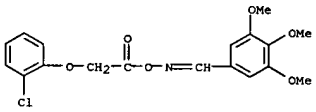
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 10 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409310-57-2 REGISTRY
ED Entered STN: 01 May 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(2-chlorophenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H18 Cl N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	849	pH 1	(1) ACD
Bioconc. Factor (BCF)	849	pH 4	(1) ACD
Bioconc. Factor (BCF)	849	pH 7	(1) ACD
Bioconc. Factor (BCF)	849	pH 8	(1) ACD
Bioconc. Factor (BCF)	849	pH 10	(1) ACD
Boiling Point (BP)	507.5+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	77.76+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	260.7+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	8		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	4345	pH 1	(1) ACD
Koc (KOC)	4345	pH 4	(1) ACD
Koc (KOC)	4345	pH 7	(1) ACD
Koc (KOC)	4345	pH 8	(1) ACD
Koc (KOC)	4345	pH 10	(1) ACD
logD (LOGD)	4.16	pH 1	(1) ACD
logD (LOGD)	4.16	pH 4	(1) ACD
logD (LOGD)	4.16	pH 7	(1) ACD
logD (LOGD)	4.16	pH 8	(1) ACD
logD (LOGD)	4.16	pH 10	(1) ACD
logP (LOGP)	4.156+/-0.608		(1) ACD

L6 ANSWER 10 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	379.79		(1) ACD
Vapor Pressure (VP)	2.02E-10 Torr	25.0 deg C	(1) ACD

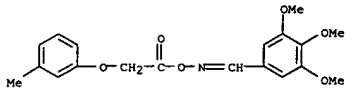
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 11 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409310-51-6 REGISTRY
ED Entered STN: 01 May 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(3-methylphenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H21 N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence Count
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	715	pH 1	(1) ACD
Bioconc. Factor (BCF)	715	pH 4	(1) ACD
Bioconc. Factor (BCF)	715	pH 7	(1) ACD
Bioconc. Factor (BCF)	715	pH 8	(1) ACD
Bioconc. Factor (BCF)	715	pH 10	(1) ACD
Boiling Point (BP)	500.4+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	76.90+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	201.6+/-49.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	8		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	3843	pH 1	(1) ACD
Koc (KOC)	3843	pH 4	(1) ACD
Koc (KOC)	3843	pH 7	(1) ACD
Koc (KOC)	3843	pH 8	(1) ACD
Koc (KOC)	3843	pH 10	(1) ACD
logD (LOGD)	4.06	pH 1	(1) ACD
logD (LOGD)	4.06	pH 4	(1) ACD
logD (LOGD)	4.06	pH 7	(1) ACD
logD (LOGD)	4.06	pH 8	(1) ACD
logD (LOGD)	4.06	pH 10	(1) ACD
logP (LOGP)	4.058+/-0.603		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD

L6 ANSWER 11 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	359.37		(1) ACD
Vapor Pressure (VP)	3.82E-10 Torr	25.0 deg C	(1) ACD

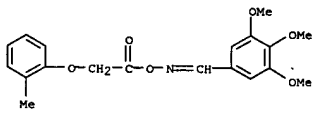
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 12 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409309-67-7 REGISTRY
ED Entered STN: 01 May 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(2-methylphenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H21 N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence Count
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	715	pH 1	(1) ACD
Bioconc. Factor (BCF)	715	pH 4	(1) ACD
Bioconc. Factor (BCF)	715	pH 7	(1) ACD
Bioconc. Factor (BCF)	715	pH 8	(1) ACD
Bioconc. Factor (BCF)	715	pH 10	(1) ACD
Boiling Point (BP)	493.0+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	76.00+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	196.9+/-46.7 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	8		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	3843	pH 1	(1) ACD
Koc (KOC)	3843	pH 4	(1) ACD
Koc (KOC)	3843	pH 7	(1) ACD
Koc (KOC)	3843	pH 8	(1) ACD
Koc (KOC)	3843	pH 10	(1) ACD
logD (LOGD)	4.06	pH 1	(1) ACD
logD (LOGD)	4.06	pH 4	(1) ACD
logD (LOGD)	4.06	pH 7	(1) ACD
logD (LOGD)	4.06	pH 8	(1) ACD
logD (LOGD)	4.06	pH 10	(1) ACD
logP (LOGP)	4.058+/-0.603		(1) ACD

L6 ANSWER 12 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	359.37		(1) ACD
Vapor Pressure (VP)	7.34E-10 Torr	25.0 deg C	(1) ACD

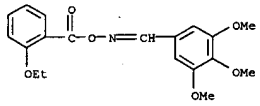
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 13 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409308-82-3 REGISTRY
ED Entered STN: 01 May 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-ethoxybenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H21 N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	640	pH 1	(1) ACD
Bioconc. Factor (BCF)	640	pH 4	(1) ACD
Bioconc. Factor (BCF)	640	pH 7	(1) ACD
Bioconc. Factor (BCF)	640	pH 8	(1) ACD
Bioconc. Factor (BCF)	640	pH 10	(1) ACD
Boiling Point (BP)	498.4+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	76.65+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	200.3+/-46.7 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	8		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	3552	pH 1	(1) ACD
Koc (KOC)	3552	pH 4	(1) ACD
Koc (KOC)	3552	pH 7	(1) ACD
Koc (KOC)	3552	pH 8	(1) ACD
Koc (KOC)	3552	pH 10	(1) ACD
logD (LOGD)	4.00	pH 1	(1) ACD
logD (LOGD)	4.00	pH 4	(1) ACD
logD (LOGD)	4.00	pH 7	(1) ACD
logD (LOGD)	4.00	pH 8	(1) ACD
logD (LOGD)	4.00	pH 10	(1) ACD
logP (LOGP)	3.995+/-0.594		(1) ACD

L6 ANSWER 13 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	359.37		(1) ACD
Vapor Pressure (VP)	4.57E-10 Torr	25.0 deg C	(1) ACD

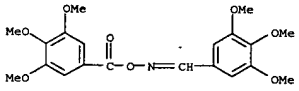
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 14 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409308-34-5 REGISTRY
ED Entered STN: 01 May 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(3,4,5-trimethoxybenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H23 N O8
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	565	pH 1	(1) ACD
Bioconc. Factor (BCF)	565	pH 4	(1) ACD
Bioconc. Factor (BCF)	565	pH 7	(1) ACD
Bioconc. Factor (BCF)	565	pH 8	(1) ACD
Bioconc. Factor (BCF)	565	pH 10	(1) ACD
Boiling Point (BP)	546.9+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	82.61+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	215.0+/-49.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	9		(1) ACD
H acceptors (HAC)	9		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	3247	pH 1	(1) ACD
Koc (KOC)	3247	pH 4	(1) ACD
Koc (KOC)	3247	pH 7	(1) ACD
Koc (KOC)	3247	pH 8	(1) ACD
Koc (KOC)	3247	pH 10	(1) ACD
logD (LOGD)	3.92	pH 1	(1) ACD
logD (LOGD)	3.92	pH 4	(1) ACD
logD (LOGD)	3.92	pH 7	(1) ACD
logD (LOGD)	3.92	pH 8	(1) ACD
logD (LOGD)	3.92	pH 10	(1) ACD
logP (LOGP)	3.924+/-0.612		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD

L6 ANSWER 14 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	405.40		(1) ACD
Vapor Pressure (VP)	5.15E-12 Torr	25.0 deg C	(1) ACD

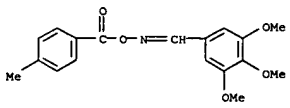
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 15 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409307-85-3 REGISTRY
ED Entered STN: 01 May 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(4-methylbenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H19 N O5
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	906	pH 1	(1) ACD
Bioconc. Factor (BCF)	906	pH 4	(1) ACD
Bioconc. Factor (BCF)	906	pH 7	(1) ACD
Bioconc. Factor (BCF)	906	pH 8	(1) ACD
Bioconc. Factor (BCF)	906	pH 10	(1) ACD
Boiling Point (BP)	466.2+/-50.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	72.80+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	191.8+/-44.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	6		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	4554	pH 1	(1) ACD
Koc (KOC)	4554	pH 4	(1) ACD
Koc (KOC)	4554	pH 7	(1) ACD
Koc (KOC)	4554	pH 8	(1) ACD
Koc (KOC)	4554	pH 10	(1) ACD
logD (LOGD)	4.19	pH 1	(1) ACD
logD (LOGD)	4.19	pH 4	(1) ACD
logD (LOGD)	4.19	pH 7	(1) ACD
logD (LOGD)	4.19	pH 8	(1) ACD
logD (LOGD)	4.19	pH 10	(1) ACD
logP (LOGP)	4.194+/-0.585		(1) ACD

L6 ANSWER 15 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	329.35		(1) ACD
Vapor Pressure (VP)	7.22E-09 Torr	25.0 deg C	(1) ACD

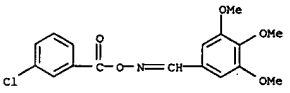
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 16 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409125-17-3 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(3-chlorobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H16 Cl N O5
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1631	pH 1	(1) ACD
Bioconc. Factor (BCF)	1631	pH 4	(1) ACD
Bioconc. Factor (BCF)	1631	pH 7	(1) ACD
Bioconc. Factor (BCF)	1631	pH 8	(1) ACD
Bioconc. Factor (BCF)	1631	pH 10	(1) ACD
Boiling Point (BP)	478.6+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	74.27+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	243.2+/-56.7 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	6		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	6937	pH 1	(1) ACD
Koc (KOC)	6937	pH 4	(1) ACD
Koc (KOC)	6937	pH 7	(1) ACD
Koc (KOC)	6937	pH 8	(1) ACD
Koc (KOC)	6937	pH 10	(1) ACD
logD (LOGD)	4.53	pH 1	(1) ACD
logD (LOGD)	4.53	pH 4	(1) ACD
logD (LOGD)	4.53	pH 7	(1) ACD
logD (LOGD)	4.53	pH 8	(1) ACD
logD (LOGD)	4.53	pH 10	(1) ACD
logP (LOGP)	4.530+/-0.592		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

L6 ANSWER 16 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	349.77		(1) ACD
Vapor Pressure (VP)	2.55E-09 Torr	25.0 deg C	(1) ACD

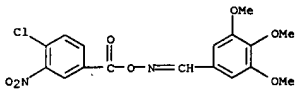
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 17 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409124-54-5 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(4-chloro-3-nitrobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H15 Cl N2 O7
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	917	pH 1	(1) ACD
Bioconc. Factor (BCF)	917	pH 4	(1) ACD
Bioconc. Factor (BCF)	917	pH 7	(1) ACD
Bioconc. Factor (BCF)	917	pH 8	(1) ACD
Bioconc. Factor (BCF)	917	pH 10	(1) ACD
Boiling Point (BP)	541.7+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	81.96+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	281.4+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	9		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	4594	pH 1	(1) ACD
Koc (KOC)	4594	pH 4	(1) ACD
Koc (KOC)	4594	pH 7	(1) ACD
Koc (KOC)	4594	pH 8	(1) ACD
Koc (KOC)	4594	pH 10	(1) ACD
logD (LOGD)	4.20	pH 1	(1) ACD
logD (LOGD)	4.20	pH 4	(1) ACD
logD (LOGD)	4.20	pH 7	(1) ACD
logD (LOGD)	4.20	pH 8	(1) ACD
logD (LOGD)	4.20	pH 10	(1) ACD
logP (LOGP)	4.201+/-0.601		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD

L6 ANSWER 17 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	394.76		(1) ACD
Vapor Pressure (VP)	8.51E-12 Torr	25.0 deg C	(1) ACD

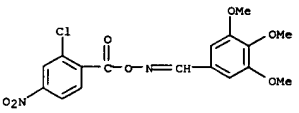
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 18 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409124-36-3 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-chloro-4-nitrobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H15 Cl N2 O7
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	604	pH 1	(1) ACD
Bioconc. Factor (BCF)	604	pH 4	(1) ACD
Bioconc. Factor (BCF)	604	pH 7	(1) ACD
Bioconc. Factor (BCF)	604	pH 8	(1) ACD
Bioconc. Factor (BCF)	604	pH 10	(1) ACD
Boiling Point (BP)	546.6+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	82.58+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	284.4+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	9		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	3407	pH 1	(1) ACD
Koc (KOC)	3407	pH 4	(1) ACD
Koc (KOC)	3407	pH 7	(1) ACD
Koc (KOC)	3407	pH 8	(1) ACD
Koc (KOC)	3407	pH 10	(1) ACD
logD (LOGD)	3.96	pH 1	(1) ACD
logD (LOGD)	3.96	pH 4	(1) ACD
logD (LOGD)	3.96	pH 7	(1) ACD
logD (LOGD)	3.96	pH 8	(1) ACD
logD (LOGD)	3.96	pH 10	(1) ACD
logP (LOGP)	3.962+/-0.604		(1) ACD

L6 ANSWER 18 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	394.76		(1) ACD
Vapor Pressure (VP)	5.28E-12 Torr	25.0 deg C	(1) ACD

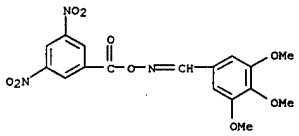
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 19 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409123-19-9 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(3,5-dinitrobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H15 N3 O9
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence Count
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	266	pH 1	(1) ACD
Bioconc. Factor (BCF)	266	pH 4	(1) ACD
Bioconc. Factor (BCF)	266	pH 7	(1) ACD
Bioconc. Factor (BCF)	266	pH 8	(1) ACD
Bioconc. Factor (BCF)	266	pH 10	(1) ACD
Boiling Point (BP)	558.2+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	84.02+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	291.4+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	8		(1) ACD
H acceptors (HAC)	12		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	1895	pH 1	(1) ACD
Koc (KOC)	1895	pH 4	(1) ACD
Koc (KOC)	1895	pH 7	(1) ACD
Koc (KOC)	1895	pH 8	(1) ACD
Koc (KOC)	1895	pH 10	(1) ACD
logD (LOGD)	3.49	pH 1	(1) ACD
logD (LOGD)	3.49	pH 4	(1) ACD
logD (LOGD)	3.49	pH 7	(1) ACD
logD (LOGD)	3.49	pH 8	(1) ACD
logD (LOGD)	3.49	pH 10	(1) ACD

L6 ANSWER 19 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

logP (LOGP)	3.494+/-0.601		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	405.32		(1) ACD
Vapor Pressure (VP)	1.71E-12 Torr	25.0 deg C	(1) ACD

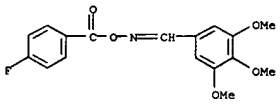
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 20 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409122-57-2 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(4-fluorobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H16 F N O5
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence Count
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	596	pH 1	(1) ACD
Bioconc. Factor (BCF)	596	pH 4	(1) ACD
Bioconc. Factor (BCF)	596	pH 7	(1) ACD
Bioconc. Factor (BCF)	596	pH 8	(1) ACD
Bioconc. Factor (BCF)	596	pH 10	(1) ACD
Boiling Point (BP)	452.6+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	71.19+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	227.5+/-56.7 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	6		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	3374	pH 1	(1) ACD
Koc (KOC)	3374	pH 4	(1) ACD
Koc (KOC)	3374	pH 7	(1) ACD
Koc (KOC)	3374	pH 8	(1) ACD
Koc (KOC)	3374	pH 10	(1) ACD
logD (LOGD)	3.95	pH 1	(1) ACD
logD (LOGD)	3.95	pH 4	(1) ACD
logD (LOGD)	3.95	pH 7	(1) ACD
logD (LOGD)	3.95	pH 8	(1) ACD
logD (LOGD)	3.95	pH 10	(1) ACD
logP (LOGP)	3.954+/-0.621		(1) ACD

L6 ANSWER 20 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	333.31		(1) ACD
Vapor Pressure (VP)	2.21E-08 Torr	25.0 deg C	(1) ACD

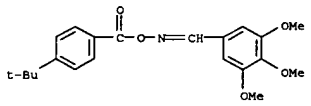
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 21 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409122-03-8 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[4-(1,1-dimethylethyl)benzoyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H25 N O5
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	7775	pH 1	(1) ACD
Bioconc. Factor (BCF)	7775	pH 4	(1) ACD
Bioconc. Factor (BCF)	7775	pH 7	(1) ACD
Bioconc. Factor (BCF)	7775	pH 8	(1) ACD
Bioconc. Factor (BCF)	7775	pH 10	(1) ACD
Boiling Point (BP)	486.5+/-50.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	75.22+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	179.2+/-44.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	21210	pH 1	(1) ACD
Koc (KOC)	21210	pH 4	(1) ACD
Koc (KOC)	21210	pH 7	(1) ACD
Koc (KOC)	21210	pH 8	(1) ACD
Koc (KOC)	21210	pH 10	(1) ACD
logD (LOGD)	5.42	pH 1	(1) ACD
logD (LOGD)	5.42	pH 4	(1) ACD
logD (LOGD)	5.42	pH 7	(1) ACD
logD (LOGD)	5.42	pH 8	(1) ACD
logD (LOGD)	5.42	pH 10	(1) ACD
logP (LOGP)	5.422+/-0.591		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

L6 ANSWER 21 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	371.43		(1) ACD
Vapor Pressure (VP)	1.28E-09 Torr	25.0 deg C	(1) ACD

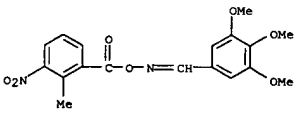
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 22 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409121-98-8 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-methyl-3-nitrobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H18 N2 O7
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	776	pH 1	(1) ACD
Bioconc. Factor (BCF)	776	pH 4	(1) ACD
Bioconc. Factor (BCF)	776	pH 7	(1) ACD
Bioconc. Factor (BCF)	776	pH 8	(1) ACD
Bioconc. Factor (BCF)	776	pH 10	(1) ACD
Boiling Point (BP)	524.2+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	79.81+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	270.8+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	9		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	4074	pH 1	(1) ACD
Koc (KOC)	4074	pH 4	(1) ACD
Koc (KOC)	4074	pH 7	(1) ACD
Koc (KOC)	4074	pH 8	(1) ACD
Koc (KOC)	4074	pH 10	(1) ACD
logD (LOGD)	4.10	pH 1	(1) ACD
logD (LOGD)	4.10	pH 4	(1) ACD
logD (LOGD)	4.10	pH 7	(1) ACD
logD (LOGD)	4.10	pH 8	(1) ACD
logD (LOGD)	4.10	pH 10	(1) ACD
logP (LOGP)	4.105+/-0.594		(1) ACD

L6 ANSWER 22 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	374.34		(1) ACD
Vapor Pressure (VP)	4.40E-11 Torr	25.0 deg C	(1) ACD

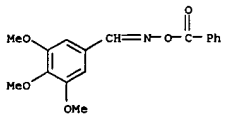
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 23 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409121-91-1 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-benzoyloxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H17 N O5
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	405	pH 1	(1) ACD
Bioconc. Factor (BCF)	405	pH 4	(1) ACD
Bioconc. Factor (BCF)	405	pH 7	(1) ACD
Bioconc. Factor (BCF)	405	pH 8	(1) ACD
Bioconc. Factor (BCF)	405	pH 10	(1) ACD
Boiling Point (BP)	443.4+/-50.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	70.10+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	185.5+/-44.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	6		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	2559	pH 1	(1) ACD
Koc (KOC)	2559	pH 4	(1) ACD
Koc (KOC)	2559	pH 7	(1) ACD
Koc (KOC)	2559	pH 8	(1) ACD
Koc (KOC)	2559	pH 10	(1) ACD
logD (LOGD)	3.73	pH 1	(1) ACD
logD (LOGD)	3.73	pH 4	(1) ACD
logD (LOGD)	3.73	pH 7	(1) ACD
logD (LOGD)	3.73	pH 8	(1) ACD
logD (LOGD)	3.73	pH 10	(1) ACD
logP (LOGP)	3.734+/-0.584		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

L6 ANSWER 23 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	315.32		(1) ACD
Vapor Pressure (VP)	4.65E-08 Torr	25.0 deg C	(1) ACD

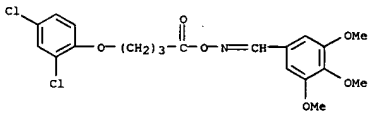
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 24 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409121-41-1 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[4-(2,4-dichlorophenoxy)-1-oxobutyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H21 Cl2 N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	8705	pH 1	(1) ACD
Bioconc. Factor (BCF)	8705	pH 4	(1) ACD
Bioconc. Factor (BCF)	8705	pH 7	(1) ACD
Bioconc. Factor (BCF)	8705	pH 8	(1) ACD
Bioconc. Factor (BCF)	8705	pH 10	(1) ACD
Boiling Point (BP)	560.2+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	84.27+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	292.6+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	10		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	22997	pH 1	(1) ACD
Koc (KOC)	22997	pH 4	(1) ACD
Koc (KOC)	22997	pH 7	(1) ACD
Koc (KOC)	22997	pH 8	(1) ACD
Koc (KOC)	22997	pH 10	(1) ACD
logD (LOGD)	5.49	pH 1	(1) ACD
logD (LOGD)	5.49	pH 4	(1) ACD
logD (LOGD)	5.49	pH 7	(1) ACD
logD (LOGD)	5.49	pH 8	(1) ACD
logD (LOGD)	5.49	pH 10	(1) ACD
logP (LOGP)	5.487+/-0.606		(1) ACD

L6 ANSWER 24 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	442.29		(1) ACD
Vapor Pressure (VP)	1.40E-12 Torr	25.0 deg C	(1) ACD

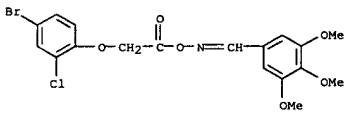
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 25 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409120-61-2 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(4-bromo-2-chlorophenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H17 Br Cl N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence Count
EA	ES	SZ	RF	RID	
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	5003	pH 1	(1) ACD
Bioconc. Factor (BCF)	5003	pH 4	(1) ACD
Bioconc. Factor (BCF)	5003	pH 7	(1) ACD
Bioconc. Factor (BCF)	5003	pH 8	(1) ACD
Bioconc. Factor (BCF)	5003	pH 10	(1) ACD
Boiling Point (BP)	545.0+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	82.37+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	283.4+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	8		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	15470	pH 1	(1) ACD
Koc (KOC)	15470	pH 4	(1) ACD
Koc (KOC)	15470	pH 7	(1) ACD
Koc (KOC)	15470	pH 8	(1) ACD
Koc (KOC)	15470	pH 10	(1) ACD
logD (LOGD)	5.17	pH 1	(1) ACD
logD (LOGD)	5.17	pH 4	(1) ACD
logD (LOGD)	5.17	pH 7	(1) ACD
logD (LOGD)	5.17	pH 8	(1) ACD
logD (LOGD)	5.17	pH 10	(1) ACD
logP (LOGP)	5.170+/-0.641		(1) ACD

L6 ANSWER 25 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	458.69		(1) ACD
Vapor Pressure (VP)	6.18E-12 Torr	25.0 deg C	(1) ACD

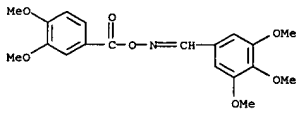
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 26 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409119-87-5 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(3,4-dimethoxybenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H21 N O7
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence Count
EA	ES	SZ	RF	RID	
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	614	pH 1	(1) ACD
Bioconc. Factor (BCF)	614	pH 4	(1) ACD
Bioconc. Factor (BCF)	614	pH 7	(1) ACD
Bioconc. Factor (BCF)	614	pH 8	(1) ACD
Bioconc. Factor (BCF)	614	pH 10	(1) ACD
Boiling Point (BP)	515.7+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	78.77+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	207.8+/-49.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	8		(1) ACD
H acceptors (HAC)	8		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	3448	pH 1	(1) ACD
Koc (KOC)	3448	pH 4	(1) ACD
Koc (KOC)	3448	pH 7	(1) ACD
Koc (KOC)	3448	pH 8	(1) ACD
Koc (KOC)	3448	pH 10	(1) ACD
logD (LOGD)	3.97	pH 1	(1) ACD
logD (LOGD)	3.97	pH 4	(1) ACD
logD (LOGD)	3.97	pH 7	(1) ACD
logD (LOGD)	3.97	pH 8	(1) ACD
logD (LOGD)	3.97	pH 10	(1) ACD
logP (LOGP)	3.972+/-0.602		(1) ACD

L6 ANSWER 26 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	375.37		(1) ACD
Vapor Pressure (VP)	9.60E-11 Torr	25.0 deg C	(1) ACD

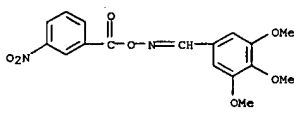
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 27 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409119-23-9 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(3-nitrobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H16 N2 O7
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	347	pH 1	(1) ACD
Bioconc. Factor (BCF)	347	pH 4	(1) ACD
Bioconc. Factor (BCF)	347	pH 7	(1) ACD
Bioconc. Factor (BCF)	347	pH 8	(1) ACD
Bioconc. Factor (BCF)	347	pH 10	(1) ACD
Boiling Point (BP)	509.6+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	78.01+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	262.0+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	9		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	2289	pH 1	(1) ACD
Koc (KOC)	2289	pH 4	(1) ACD
Koc (KOC)	2289	pH 7	(1) ACD
Koc (KOC)	2289	pH 8	(1) ACD
Koc (KOC)	2289	pH 10	(1) ACD
logD (LOGD)	3.64	pH 1	(1) ACD
logD (LOGD)	3.64	pH 4	(1) ACD
logD (LOGD)	3.64	pH 7	(1) ACD
logD (LOGD)	3.64	pH 8	(1) ACD
logD (LOGD)	3.64	pH 10	(1) ACD
logP (LOGP)	3.645+/-0.592		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

L6 ANSWER 27 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	360.32		(1) ACD
Vapor Pressure (VP)	1.68E-10 Torr	25.0 deg C	(1) ACD

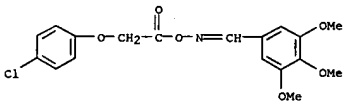
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 28 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409119-16-0 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(4-chlorophenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H18 Cl N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1062	pH 1	(1) ACD
Bioconc. Factor (BCF)	1062	pH 4	(1) ACD
Bioconc. Factor (BCF)	1062	pH 7	(1) ACD
Bioconc. Factor (BCF)	1062	pH 8	(1) ACD
Bioconc. Factor (BCF)	1062	pH 10	(1) ACD
Boiling Point (BP)	509.4+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	77.99+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	261.9+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	8		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	5103	pH 1	(1) ACD
Koc (KOC)	5103	pH 4	(1) ACD
Koc (KOC)	5103	pH 7	(1) ACD
Koc (KOC)	5103	pH 8	(1) ACD
Koc (KOC)	5103	pH 10	(1) ACD
logD (LOGD)	4.28	pH 1	(1) ACD
logD (LOGD)	4.28	pH 4	(1) ACD
logD (LOGD)	4.28	pH 7	(1) ACD
logD (LOGD)	4.28	pH 8	(1) ACD
logD (LOGD)	4.28	pH 10	(1) ACD
logP (LOGP)	4.285+/-0.608		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

L6 ANSWER 28 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	379.79		(1) ACD
Vapor Pressure (VP)	1.70E-10 Torr	25.0 deg C	(1) ACD

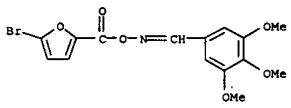
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 29 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409119-14-8 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(5-bromo-2-furanyl)carbonyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H14 Br N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C4O	OC4	5	C4O	16.138.5	1
C6	C6	6	C6	46.150.18	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	454	pH 1	(1) ACD
Bioconc. Factor (BCF)	454	pH 4	(1) ACD
Bioconc. Factor (BCF)	454	pH 7	(1) ACD
Bioconc. Factor (BCF)	454	pH 8	(1) ACD
Bioconc. Factor (BCF)	454	pH 10	(1) ACD
Boiling Point (BP)	466.9+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	72.88+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	236.2+/-56.7 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	6		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	2776	pH 1	(1) ACD
Koc (KOC)	2776	pH 4	(1) ACD
Koc (KOC)	2776	pH 7	(1) ACD
Koc (KOC)	2776	pH 8	(1) ACD
Koc (KOC)	2776	pH 10	(1) ACD
logD (LOGD)	3.80	pH 1	(1) ACD
logD (LOGD)	3.80	pH 4	(1) ACD
logD (LOGD)	3.80	pH 7	(1) ACD
logD (LOGD)	3.80	pH 8	(1) ACD
logD (LOGD)	3.80	pH 10	(1) ACD
logP (LOGP)	3.799+/-0.641		(1) ACD

L6 ANSWER 29 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	384.18		(1) ACD
Vapor Pressure (VP)	6.81E-09 Torr	25.0 deg C	(1) ACD

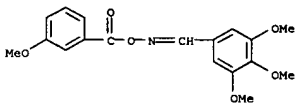
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 30 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409118-77-0 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(3-methoxybenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H19 N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	541	pH 1	(1) ACD
Bioconc. Factor (BCF)	541	pH 4	(1) ACD
Bioconc. Factor (BCF)	541	pH 7	(1) ACD
Bioconc. Factor (BCF)	541	pH 8	(1) ACD
Bioconc. Factor (BCF)	541	pH 10	(1) ACD
Boiling Point (BP)	486.0+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	75.16+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	201.0+/-46.7 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	3148	pH 1	(1) ACD
Koc (KOC)	3148	pH 4	(1) ACD
Koc (KOC)	3148	pH 7	(1) ACD
Koc (KOC)	3148	pH 8	(1) ACD
Koc (KOC)	3148	pH 10	(1) ACD
logD (LOGD)	3.90	pH 1	(1) ACD
logD (LOGD)	3.90	pH 4	(1) ACD
logD (LOGD)	3.90	pH 7	(1) ACD
logD (LOGD)	3.90	pH 8	(1) ACD
logD (LOGD)	3.90	pH 10	(1) ACD
logP (LOGP)	3.899+/-0.593		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

L6 ANSWER 30 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	345.35		(1) ACD
Vapor Pressure (VP)	1.35E-09 Torr	25.0 deg C	(1) ACD

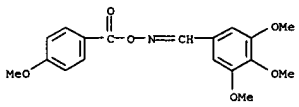
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 31 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409118-69-0 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(4-methoxybenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H19 N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	542	pH 1	(1) ACD
Bioconc. Factor (BCF)	542	pH 4	(1) ACD
Bioconc. Factor (BCF)	542	pH 7	(1) ACD
Bioconc. Factor (BCF)	542	pH 8	(1) ACD
Bioconc. Factor (BCF)	542	pH 10	(1) ACD
Boiling Point (BP)	486.7+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	75.24+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	201.5+/-46.7 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	3152	pH 1	(1) ACD
Koc (KOC)	3152	pH 4	(1) ACD
Koc (KOC)	3152	pH 7	(1) ACD
Koc (KOC)	3152	pH 8	(1) ACD
Koc (KOC)	3152	pH 10	(1) ACD
logD (LOGD)	3.90	pH 1	(1) ACD
logD (LOGD)	3.90	pH 4	(1) ACD
logD (LOGD)	3.90	pH 7	(1) ACD
logD (LOGD)	3.90	pH 8	(1) ACD
logD (LOGD)	3.90	pH 10	(1) ACD
logP (LOGP)	3.900+/-0.593		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

L6 ANSWER 31 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	345.35		(1) ACD
Vapor Pressure (VP)	1.27E-09 Torr	25.0 deg C	(1) ACD

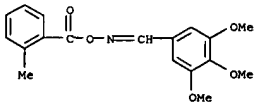
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 32 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409118-51-0 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-methylbenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H19 N O5
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	906	pH 1	(1) ACD
Bioconc. Factor (BCF)	906	pH 4	(1) ACD
Bioconc. Factor (BCF)	906	pH 7	(1) ACD
Bioconc. Factor (BCF)	906	pH 8	(1) ACD
Bioconc. Factor (BCF)	906	pH 10	(1) ACD
Boiling Point (BP)	464.9+/-50.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	72.64+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	191.0+/-44.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	6		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	4554	pH 1	(1) ACD
Koc (KOC)	4554	pH 4	(1) ACD
Koc (KOC)	4554	pH 7	(1) ACD
Koc (KOC)	4554	pH 8	(1) ACD
Koc (KOC)	4554	pH 10	(1) ACD
logD (LOGD)	4.19	pH 1	(1) ACD
logD (LOGD)	4.19	pH 4	(1) ACD
logD (LOGD)	4.19	pH 7	(1) ACD
logD (LOGD)	4.19	pH 8	(1) ACD
logD (LOGD)	4.19	pH 10	(1) ACD
logP (LOGP)	4.194+/-0.585		(1) ACD

L6 ANSWER 32 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	329.35		(1) ACD
Vapor Pressure (VP)	8.06E-09 Torr	25.0 deg C	(1) ACD

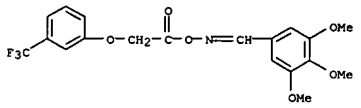
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 33 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409118-25-8 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-,
O-[[3-(trifluoromethyl)phenoxy]acetyl]oxi
me (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H18 F3 N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	2349	pH 1	(1) ACD
Bioconc. Factor (BCF)	2349	pH 4	(1) ACD
Bioconc. Factor (BCF)	2349	pH 7	(1) ACD
Bioconc. Factor (BCF)	2349	pH 8	(1) ACD
Bioconc. Factor (BCF)	2349	pH 10	(1) ACD
Boiling Point (BP)	490.0+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	75.64+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	250.1+/-56.7 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	8		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	9004	pH 1	(1) ACD
Koc (KOC)	9004	pH 4	(1) ACD
Koc (KOC)	9004	pH 7	(1) ACD
Koc (KOC)	9004	pH 8	(1) ACD
Koc (KOC)	9004	pH 10	(1) ACD
logD (LOGD)	4.74	pH 1	(1) ACD
logD (LOGD)	4.74	pH 4	(1) ACD
logD (LOGD)	4.74	pH 7	(1) ACD
logD (LOGD)	4.74	pH 8	(1) ACD
logD (LOGD)	4.74	pH 10	(1) ACD
logP (LOGP)	4.738+/-0.628		(1) ACD

L6 ANSWER 33 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	413.34		(1) ACD
Vapor Pressure (VP)	9.50E-10 Torr	25.0 deg C	(1) ACD

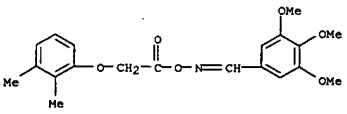
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 34 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409118-12-3 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(2,3-dimethylphenoxy)acetyl]oxime
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H23 N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1599	pH 1	(1) ACD
Bioconc. Factor (BCF)	1599	pH 4	(1) ACD
Bioconc. Factor (BCF)	1599	pH 7	(1) ACD
Bioconc. Factor (BCF)	1599	pH 8	(1) ACD
Bioconc. Factor (BCF)	1599	pH 10	(1) ACD
Boiling Point (BP)	512.4+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	78.36+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	200.7+/-49.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	8		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	6839	pH 1	(1) ACD
Koc (KOC)	6839	pH 4	(1) ACD
Koc (KOC)	6839	pH 7	(1) ACD
Koc (KOC)	6839	pH 8	(1) ACD
Koc (KOC)	6839	pH 10	(1) ACD
logD (LOGD)	4.52	pH 1	(1) ACD
logD (LOGD)	4.52	pH 4	(1) ACD
logD (LOGD)	4.52	pH 7	(1) ACD
logD (LOGD)	4.52	pH 8	(1) ACD
logD (LOGD)	4.52	pH 10	(1) ACD
logP (LOGP)	4.518+/-0.604		(1) ACD

L6 ANSWER 34 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	373.40		(1) ACD
Vapor Pressure (VP)	1.30E-10 Torr	25.0 deg C	(1) ACD

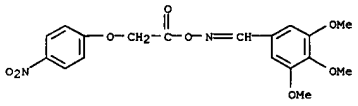
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 35 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409117-91-5 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(4-nitrophenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H18 N2 O8
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	267	pH 1	(1) ACD
Bioconc. Factor (BCF)	267	pH 4	(1) ACD
Bioconc. Factor (BCF)	267	pH 7	(1) ACD
Bioconc. Factor (BCF)	267	pH 8	(1) ACD
Bioconc. Factor (BCF)	267	pH 10	(1) ACD
Boiling Point (BP)	561.7+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	84.46+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	293.5+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	9		(1) ACD
H acceptors (HAC)	10		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	1897	pH 1	(1) ACD
Koc (KOC)	1897	pH 4	(1) ACD
Koc (KOC)	1897	pH 7	(1) ACD
Koc (KOC)	1897	pH 8	(1) ACD
Koc (KOC)	1897	pH 10	(1) ACD
logD (LOGD)	3.49	pH 1	(1) ACD
logD (LOGD)	3.49	pH 4	(1) ACD
logD (LOGD)	3.49	pH 7	(1) ACD
logD (LOGD)	3.49	pH 8	(1) ACD
logD (LOGD)	3.49	pH 10	(1) ACD
logP (LOGP)	3.495+/-0.609		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

L6 ANSWER 35 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	390.34		(1) ACD
Vapor Pressure (VP)	1.21E-12 Torr	25.0 deg C	(1) ACD

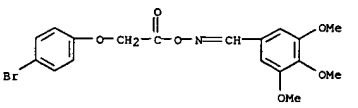
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 36 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409117-26-6 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(4-bromophenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H18 Br N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1864	pH 1	(1) ACD
Bioconc. Factor (BCF)	1864	pH 4	(1) ACD
Bioconc. Factor (BCF)	1864	pH 7	(1) ACD
Bioconc. Factor (BCF)	1864	pH 8	(1) ACD
Bioconc. Factor (BCF)	1864	pH 10	(1) ACD
Boiling Point (BP)	524.8+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	79.88+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	271.2+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	8		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	7632	pH 1	(1) ACD
Koc (KOC)	7632	pH 4	(1) ACD
Koc (KOC)	7632	pH 7	(1) ACD
Koc (KOC)	7632	pH 8	(1) ACD
Koc (KOC)	7632	pH 10	(1) ACD
logD (LOGD)	4.61	pH 1	(1) ACD
logD (LOGD)	4.61	pH 4	(1) ACD
logD (LOGD)	4.61	pH 7	(1) ACD
logD (LOGD)	4.61	pH 8	(1) ACD
logD (LOGD)	4.61	pH 10	(1) ACD
logP (LOGP)	4.606+/-0.635		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

L6 ANSWER 36 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	424.24		(1) ACD
Vapor Pressure (VP)	4.16E-11 Torr	25.0 deg C	(1) ACD

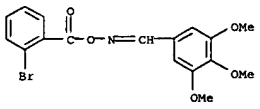
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 37 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409116-32-1 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-bromobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H16 Br N O5
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	747	pH 1	(1) ACD
Bioconc. Factor (BCF)	747	pH 4	(1) ACD
Bioconc. Factor (BCF)	747	pH 7	(1) ACD
Bioconc. Factor (BCF)	747	pH 8	(1) ACD
Bioconc. Factor (BCF)	747	pH 10	(1) ACD
Boiling Point (BP)	492.4+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	75.93+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	251.6+/-56.7 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	6		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	3966	pH 1	(1) ACD
Koc (KOC)	3966	pH 4	(1) ACD
Koc (KOC)	3966	pH 7	(1) ACD
Koc (KOC)	3966	pH 8	(1) ACD
Koc (KOC)	3966	pH 10	(1) ACD
logD (LOGD)	4.08	pH 1	(1) ACD
logD (LOGD)	4.08	pH 4	(1) ACD
logD (LOGD)	4.08	pH 7	(1) ACD
logD (LOGD)	4.08	pH 8	(1) ACD
logD (LOGD)	4.08	pH 10	(1) ACD
logP (LOGP)	4.083+/-0.624		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

L6 ANSWER 37 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	394.22		(1) ACD
Vapor Pressure (VP)	7.73E-10 Torr	25.0 deg C	(1) ACD

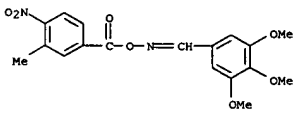
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris,V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 38 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409115-93-1 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(3-methyl-4-nitrobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H18 N2 O7
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	846	pH 1	(1) ACD
Bioconc. Factor (BCF)	846	pH 4	(1) ACD
Bioconc. Factor (BCF)	846	pH 7	(1) ACD
Bioconc. Factor (BCF)	846	pH 8	(1) ACD
Bioconc. Factor (BCF)	846	pH 10	(1) ACD
Boiling Point (BP)	540.1+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	81.77+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	280.5+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	9		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	4337	pH 1	(1) ACD
Koc (KOC)	4337	pH 4	(1) ACD
Koc (KOC)	4337	pH 7	(1) ACD
Koc (KOC)	4337	pH 8	(1) ACD
Koc (KOC)	4337	pH 10	(1) ACD
logD (LOGD)	4.15	pH 1	(1) ACD
logD (LOGD)	4.15	pH 4	(1) ACD
logD (LOGD)	4.15	pH 7	(1) ACD
logD (LOGD)	4.15	pH 8	(1) ACD
logD (LOGD)	4.15	pH 10	(1) ACD
logP (LOGP)	4.155+/-0.594		(1) ACD

L6 ANSWER 38 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	374.34		(1) ACD
Vapor Pressure (VP)	9.84E-12 Torr	25.0 deg C	(1) ACD

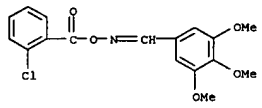
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 39 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409115-90-8 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-chlorobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H16 Cl N O5
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	548	pH 1	(1) ACD
Bioconc. Factor (BCF)	548	pH 4	(1) ACD
Bioconc. Factor (BCF)	548	pH 7	(1) ACD
Bioconc. Factor (BCF)	548	pH 8	(1) ACD
Bioconc. Factor (BCF)	548	pH 10	(1) ACD
Boiling Point (BP)	477.2+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	74.10+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	242.4+/-56.7 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	6		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	3179	pH 1	(1) ACD
Koc (KOC)	3179	pH 4	(1) ACD
Koc (KOC)	3179	pH 7	(1) ACD
Koc (KOC)	3179	pH 8	(1) ACD
Koc (KOC)	3179	pH 10	(1) ACD
logD (LOGD)	3.91	pH 1	(1) ACD
logD (LOGD)	3.91	pH 4	(1) ACD
logD (LOGD)	3.91	pH 7	(1) ACD
logD (LOGD)	3.91	pH 8	(1) ACD
logD (LOGD)	3.91	pH 10	(1) ACD
logP (LOGP)	3.907+/-0.595		(1) ACD

L6 ANSWER 39 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	349.77		(1) ACD
Vapor Pressure (VP)	2.86E-09 Torr	25.0 deg C	(1) ACD

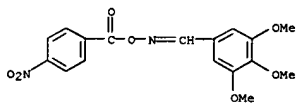
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 40 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409115-64-6 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(4-nitrobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H16 N2 O7
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	378	pH 1	(1) ACD
Bioconc. Factor (BCF)	378	pH 4	(1) ACD
Bioconc. Factor (BCF)	378	pH 7	(1) ACD
Bioconc. Factor (BCF)	378	pH 8	(1) ACD
Bioconc. Factor (BCF)	378	pH 10	(1) ACD
Boiling Point (BP)	523.3+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	79.69+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	270.3+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	9		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	2437	pH 1	(1) ACD
Koc (KOC)	2437	pH 4	(1) ACD
Koc (KOC)	2437	pH 7	(1) ACD
Koc (KOC)	2437	pH 8	(1) ACD
Koc (KOC)	2437	pH 10	(1) ACD
logD (LOGD)	3.69	pH 1	(1) ACD
logD (LOGD)	3.69	pH 4	(1) ACD
logD (LOGD)	3.69	pH 7	(1) ACD
logD (LOGD)	3.69	pH 8	(1) ACD
logD (LOGD)	3.69	pH 10	(1) ACD
logP (LOGP)	3.695+/-0.592		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

L6 ANSWER 40 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	360.32		(1) ACD
Vapor Pressure (VP)	4.78E-11 Torr	25.0 deg C	(1) ACD

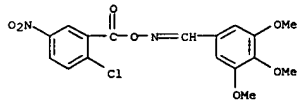
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 41 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409115-37-3 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-chloro-5-nitrobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H15 Cl N2 O7
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence Count
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	518	pH 1	(1) ACD
Bioconc. Factor (BCF)	518	pH 4	(1) ACD
Bioconc. Factor (BCF)	518	pH 7	(1) ACD
Bioconc. Factor (BCF)	518	pH 8	(1) ACD
Bioconc. Factor (BCF)	518	pH 10	(1) ACD
Boiling Point (BP)	539.5+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	81.69+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	280.1+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	9		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	3051	pH 1	(1) ACD
Koc (KOC)	3051	pH 4	(1) ACD
Koc (KOC)	3051	pH 7	(1) ACD
Koc (KOC)	3051	pH 8	(1) ACD
Koc (KOC)	3051	pH 10	(1) ACD
logD (LOGD)	3.87	pH 1	(1) ACD
logD (LOGD)	3.87	pH 4	(1) ACD
logD (LOGD)	3.87	pH 7	(1) ACD
logD (LOGD)	3.87	pH 8	(1) ACD
logD (LOGD)	3.87	pH 10	(1) ACD
logP (LOGP)	3.874+/-0.604		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

L6 ANSWER 41 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	394.76		(1) ACD
Vapor Pressure (VP)	1.05E-11 Torr	25.0 deg C	(1) ACD

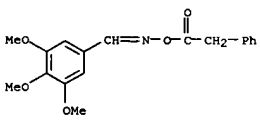
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 42 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409103-86-2 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(phenylacetyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H19 N O5
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence Count
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	423	pH 1	(1) ACD
Bioconc. Factor (BCF)	423	pH 4	(1) ACD
Bioconc. Factor (BCF)	423	pH 7	(1) ACD
Bioconc. Factor (BCF)	423	pH 8	(1) ACD
Bioconc. Factor (BCF)	423	pH 10	(1) ACD
Boiling Point (BP)	466.4+/-50.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	72.81+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	191.9+/-44.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	2638	pH 1	(1) ACD
Koc (KOC)	2638	pH 4	(1) ACD
Koc (KOC)	2638	pH 7	(1) ACD
Koc (KOC)	2638	pH 8	(1) ACD
Koc (KOC)	2638	pH 10	(1) ACD
logD (LOGD)	3.76	pH 1	(1) ACD
logD (LOGD)	3.76	pH 4	(1) ACD
logD (LOGD)	3.76	pH 7	(1) ACD
logD (LOGD)	3.76	pH 8	(1) ACD
logD (LOGD)	3.76	pH 10	(1) ACD
logP (LOGP)	3.758+/-0.589		(1) ACD

L6 ANSWER 42 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	329.35		(1) ACD
Vapor Pressure (VP)	7.13E-09 Torr	25.0 deg C	(1) ACD

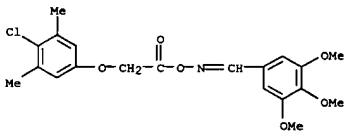
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 43 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409103-02-2 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(4-chloro-3,5-dimethylphenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H22 Cl N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	5316	pH 1	(1) ACD
Bioconc. Factor (BCF)	5316	pH 4	(1) ACD
Bioconc. Factor (BCF)	5316	pH 7	(1) ACD
Bioconc. Factor (BCF)	5316	pH 8	(1) ACD
Bioconc. Factor (BCF)	5316	pH 10	(1) ACD
Boiling Point (BP)	539.5+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	81.70+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	280.1+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	8		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	16157	pH 1	(1) ACD
Koc (KOC)	16157	pH 4	(1) ACD
Koc (KOC)	16157	pH 7	(1) ACD
Koc (KOC)	16157	pH 8	(1) ACD
Koc (KOC)	16157	pH 10	(1) ACD
logD (LOGD)	5.20	pH 1	(1) ACD
logD (LOGD)	5.20	pH 4	(1) ACD
logD (LOGD)	5.20	pH 7	(1) ACD
logD (LOGD)	5.20	pH 8	(1) ACD
logD (LOGD)	5.20	pH 10	(1) ACD

L6 ANSWER 43 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

logP (LOGP)	5.205+/-0.610		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	407.84		(1) ACD
Vapor Pressure (VP)	1.04E-11 Torr	25.0 deg C	(1) ACD

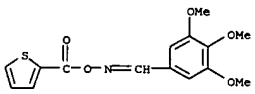
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 44 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409101-98-0 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-thienylcarbonyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H15 N O5 S
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C4S	SC4	5	C4S	16.145.3	1
C6	C6	6	C6	46.150.18	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	202	pH 1	(1) ACD
Bioconc. Factor (BCF)	202	pH 4	(1) ACD
Bioconc. Factor (BCF)	202	pH 7	(1) ACD
Bioconc. Factor (BCF)	202	pH 8	(1) ACD
Bioconc. Factor (BCF)	202	pH 10	(1) ACD
Boiling Point (BP)	450.0+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	70.88+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	225.9+/-56.7 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	6		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	1556	pH 1	(1) ACD
Koc (KOC)	1556	pH 4	(1) ACD
Koc (KOC)	1556	pH 7	(1) ACD
Koc (KOC)	1556	pH 8	(1) ACD
Koc (KOC)	1556	pH 10	(1) ACD
logD (LOGD)	3.34	pH 1	(1) ACD
logD (LOGD)	3.34	pH 4	(1) ACD
logD (LOGD)	3.34	pH 7	(1) ACD
logD (LOGD)	3.34	pH 8	(1) ACD
logD (LOGD)	3.34	pH 10	(1) ACD
logP (LOGP)	3.337+/-0.600		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

L6 ANSWER 44 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	321.35		(1) ACD
Vapor Pressure (VP)	2.74E-08 Torr	25.0 deg C	(1) ACD

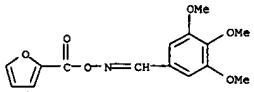
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 45 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409101-91-3 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-furanylcarbonyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H15 N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C4O	OC4	5	C4O	16.138.5	1
C6	C6	6	C6	46.150.18	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	48.9	pH 1	(1) ACD
Bioconc. Factor (BCF)	48.9	pH 4	(1) ACD
Bioconc. Factor (BCF)	48.9	pH 7	(1) ACD
Bioconc. Factor (BCF)	48.9	pH 8	(1) ACD
Bioconc. Factor (BCF)	48.9	pH 10	(1) ACD
Boiling Point (BP)	423.8+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	67.81+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	210.1+/-56.7 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	6		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	564	pH 1	(1) ACD
Koc (KOC)	564	pH 4	(1) ACD
Koc (KOC)	564	pH 7	(1) ACD
Koc (KOC)	564	pH 8	(1) ACD
Koc (KOC)	564	pH 10	(1) ACD
logD (LOGD)	2.53	pH 1	(1) ACD
logD (LOGD)	2.53	pH 4	(1) ACD
logD (LOGD)	2.53	pH 7	(1) ACD
logD (LOGD)	2.53	pH 8	(1) ACD
logD (LOGD)	2.53	pH 10	(1) ACD
logP (LOGP)	2.526+/-0.601		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

L6 ANSWER 45 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	305.28		(1) ACD
Vapor Pressure (VP)	2.18E-07 Torr	25.0 deg C	(1) ACD

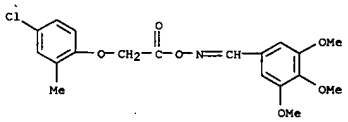
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 46 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409101-71-9 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(4-chloro-2-methylphenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H20 Cl N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	2376	pH 1	(1) ACD
Bioconc. Factor (BCF)	2376	pH 4	(1) ACD
Bioconc. Factor (BCF)	2376	pH 7	(1) ACD
Bioconc. Factor (BCF)	2376	pH 8	(1) ACD
Bioconc. Factor (BCF)	2376	pH 10	(1) ACD
Boiling Point (BP)	519.9+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	79.27+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	268.2+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	8		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	9080	pH 1	(1) ACD
Koc (KOC)	9080	pH 4	(1) ACD
Koc (KOC)	9080	pH 7	(1) ACD
Koc (KOC)	9080	pH 8	(1) ACD
Koc (KOC)	9080	pH 10	(1) ACD
logD (LOGD)	4.74	pH 1	(1) ACD
logD (LOGD)	4.74	pH 4	(1) ACD
logD (LOGD)	4.74	pH 7	(1) ACD
logD (LOGD)	4.74	pH 8	(1) ACD
logD (LOGD)	4.74	pH 10	(1) ACD

L6 ANSWER 46 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

logP (LOGP)	4.745+/-0.609		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	393.82		(1) ACD
Vapor Pressure (VP)	6.57E-11 Torr	25.0 deg C	(1) ACD

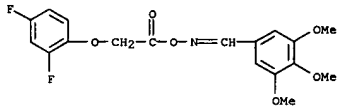
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 47 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409101-45-7 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(2,4-difluorophenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H17 F2 N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	548	pH 1	(1) ACD
Bioconc. Factor (BCF)	548	pH 4	(1) ACD
Bioconc. Factor (BCF)	548	pH 7	(1) ACD
Bioconc. Factor (BCF)	548	pH 8	(1) ACD
Bioconc. Factor (BCF)	548	pH 10	(1) ACD
Boiling Point (BP)	496.7+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	76.45+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	254.2+/-56.7 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	8		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	3178	pH 1	(1) ACD
Koc (KOC)	3178	pH 4	(1) ACD
Koc (KOC)	3178	pH 7	(1) ACD
Koc (KOC)	3178	pH 8	(1) ACD
Koc (KOC)	3178	pH 10	(1) ACD
logD (LOGD)	3.91	pH 1	(1) ACD
logD (LOGD)	3.91	pH 4	(1) ACD
logD (LOGD)	3.91	pH 7	(1) ACD
logD (LOGD)	3.91	pH 8	(1) ACD
logD (LOGD)	3.91	pH 10	(1) ACD
logP (LOGP)	3.907+/-0.664		(1) ACD

L6 ANSWER 47 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	381.33		(1) ACD
Vapor Pressure (VP)	5.28E-10 Torr	25.0 deg C	(1) ACD

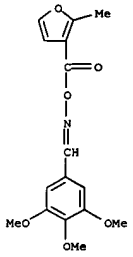
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 48 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409101-11-7 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(2-methyl-3-furanyl)carbonyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H17 N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C4O	OC4	5	C4O	16.138.5	1
C6	C6	6	C6	46.150.18	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	209	pH 1	(1) ACD
Bioconc. Factor (BCF)	209	pH 4	(1) ACD
Bioconc. Factor (BCF)	209	pH 7	(1) ACD
Bioconc. Factor (BCF)	209	pH 8	(1) ACD
Bioconc. Factor (BCF)	209	pH 10	(1) ACD
Boiling Point (BP)	442.8+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	70.04+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	221.6+/-56.7 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	6		(1) ACD

L6 ANSWER 48 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	1592	pH 1	(1) ACD
Koc (KOC)	1592	pH 4	(1) ACD
Koc (KOC)	1592	pH 7	(1) ACD
Koc (KOC)	1592	pH 8	(1) ACD
Koc (KOC)	1592	pH 10	(1) ACD
logD (LOGD)	3.35	pH 1	(1) ACD
logD (LOGD)	3.35	pH 4	(1) ACD
logD (LOGD)	3.35	pH 7	(1) ACD
logD (LOGD)	3.35	pH 8	(1) ACD
logD (LOGD)	3.35	pH 10	(1) ACD
logP (LOGP)	3.355+/-0.833		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	319.31		(1) ACD
Vapor Pressure (VP)	4.87E-08 Torr	25.0 deg C	(1) ACD

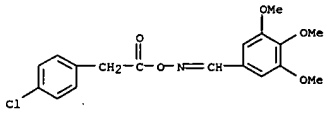
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 49 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409100-85-2 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(4-chlorophenyl)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H18 Cl N O5
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1197	pH 1	(1) ACD
Bioconc. Factor (BCF)	1197	pH 4	(1) ACD
Bioconc. Factor (BCF)	1197	pH 7	(1) ACD
Bioconc. Factor (BCF)	1197	pH 8	(1) ACD
Bioconc. Factor (BCF)	1197	pH 10	(1) ACD
Boiling Point (BP)	489.9+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	75.64+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	250.1+/-56.7 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	5559	pH 1	(1) ACD
Koc (KOC)	5559	pH 4	(1) ACD
Koc (KOC)	5559	pH 7	(1) ACD
Koc (KOC)	5559	pH 8	(1) ACD
Koc (KOC)	5559	pH 10	(1) ACD
logD (LOGD)	4.35	pH 1	(1) ACD
logD (LOGD)	4.35	pH 4	(1) ACD
logD (LOGD)	4.35	pH 7	(1) ACD
logD (LOGD)	4.35	pH 8	(1) ACD
logD (LOGD)	4.35	pH 10	(1) ACD
logP (LOGP)	4.353+/-0.595		(1) ACD

L6 ANSWER 49 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	363.79		(1) ACD
Vapor Pressure (VP)	9.55E-10 Torr	25.0 deg C	(1) ACD

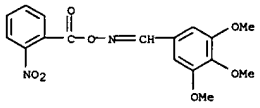
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 50 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409100-56-7 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-nitrobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H16 N2 O7
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	168	pH 1	(1) ACD
Bioconc. Factor (BCF)	168	pH 4	(1) ACD
Bioconc. Factor (BCF)	168	pH 7	(1) ACD
Bioconc. Factor (BCF)	168	pH 8	(1) ACD
Bioconc. Factor (BCF)	168	pH 10	(1) ACD
Boiling Point (BP)	517.3+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	78.95+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	266.6+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	9		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	1363	pH 1	(1) ACD
Koc (KOC)	1363	pH 4	(1) ACD
Koc (KOC)	1363	pH 7	(1) ACD
Koc (KOC)	1363	pH 8	(1) ACD
Koc (KOC)	1363	pH 10	(1) ACD
logD (LOGD)	3.23	pH 1	(1) ACD
logD (LOGD)	3.23	pH 4	(1) ACD
logD (LOGD)	3.23	pH 7	(1) ACD
logD (LOGD)	3.23	pH 8	(1) ACD
logD (LOGD)	3.23	pH 10	(1) ACD
logP (LOGP)	3.231+/-0.594		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

L6 ANSWER 50 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	360.32		(1) ACD
Vapor Pressure (VP)	8.33E-11 Torr	25.0 deg C	(1) ACD

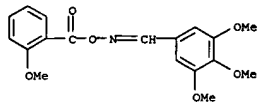
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 51 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409099-89-4 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2-methoxybenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H19 N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence Count
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	253	pH 1	(1) ACD
Bioconc. Factor (BCF)	253	pH 4	(1) ACD
Bioconc. Factor (BCF)	253	pH 7	(1) ACD
Bioconc. Factor (BCF)	253	pH 8	(1) ACD
Bioconc. Factor (BCF)	253	pH 10	(1) ACD
Boiling Point (BP)	487.8+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	75.38+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	202.2+/-46.7 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	1826	pH 1	(1) ACD
Koc (KOC)	1826	pH 4	(1) ACD
Koc (KOC)	1826	pH 7	(1) ACD
Koc (KOC)	1826	pH 8	(1) ACD
Koc (KOC)	1826	pH 10	(1) ACD
logD (LOGD)	3.46	pH 1	(1) ACD
logD (LOGD)	3.46	pH 4	(1) ACD
logD (LOGD)	3.46	pH 7	(1) ACD
logD (LOGD)	3.46	pH 8	(1) ACD
logD (LOGD)	3.46	pH 10	(1) ACD
logP (LOGP)	3.464+/-0.594		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

L6 ANSWER 51 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	345.35		(1) ACD
Vapor Pressure (VP)	1.15E-09 Torr	25.0 deg C	(1) ACD

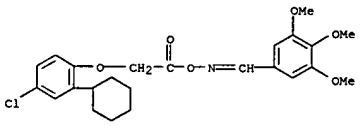
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 52 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 409099-69-0 REGISTRY
ED Entered STN: 30 Apr 2002
CN Benzaldehyde, 3,4,5-trimethoxy-, O-[(4-chloro-2-cyclohexylphenoxy)acetyl]oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C24 H28 Cl N O6
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence Count
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.1	1
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	87340	pH 1	(1) ACD
Bioconc. Factor (BCF)	87340	pH 4	(1) ACD
Bioconc. Factor (BCF)	87340	pH 7	(1) ACD
Bioconc. Factor (BCF)	87340	pH 8	(1) ACD
Bioconc. Factor (BCF)	87340	pH 10	(1) ACD
Boiling Point (BP)	578.2+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	86.54+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	303.5+/-59.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	9		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	119811	pH 1	(1) ACD
Koc (KOC)	119811	pH 4	(1) ACD
Koc (KOC)	119811	pH 7	(1) ACD
Koc (KOC)	119811	pH 8	(1) ACD
Koc (KOC)	119811	pH 10	(1) ACD
logD (LOGD)	6.80	pH 1	(1) ACD
logD (LOGD)	6.80	pH 4	(1) ACD
logD (LOGD)	6.80	pH 7	(1) ACD
logD (LOGD)	6.80	pH 8	(1) ACD

L6 ANSWER 52 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

logD (LOGD)	6.80	pH 10	(1) ACD
logP (LOGP)	6.804+/-0.609		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	461.93		(1) ACD
Vapor Pressure (VP)	2.30E-13 Torr	25.0 deg C	(1) ACD

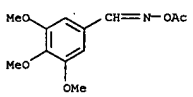
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 53 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 333438-68-9 REGISTRY
ED Entered STN: 30 Apr 2001
CN Benzaldehyde, 3,4,5-trimethoxy-, O-acetyloxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H15 N O5
SR Chemical Library
LC STN Files: CA, CAPLUS, CHEMCATS, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); USES (Uses)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	18.9	pH 1	(1) ACD
Bioconc. Factor (BCF)	18.9	pH 4	(1) ACD
Bioconc. Factor (BCF)	18.9	pH 7	(1) ACD
Bioconc. Factor (BCF)	18.9	pH 8	(1) ACD
Bioconc. Factor (BCF)	18.9	pH 10	(1) ACD
Boiling Point (BP)	358.1+/-47.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	60.35+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	155.8+/-42.7 deg C		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	285	pH 1	(1) ACD
Koc (KOC)	285	pH 4	(1) ACD
Koc (KOC)	285	pH 7	(1) ACD
Koc (KOC)	285	pH 8	(1) ACD
Koc (KOC)	285	pH 10	(1) ACD
logD (LOGD)	1.98	pH 1	(1) ACD
logD (LOGD)	1.98	pH 4	(1) ACD
logD (LOGD)	1.98	pH 7	(1) ACD
logD (LOGD)	1.98	pH 8	(1) ACD
logD (LOGD)	1.98	pH 10	(1) ACD
logP (LOGP)	1.981+/-0.584		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD

L6 ANSWER 53 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)
Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 7 | (1) ACD
Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 8 | (1) ACD
Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 10 | (1) ACD
Molecular Weight (MW) | 253.25 | | (1) ACD
Vapor Pressure (VP) | 2.61E-05 Torr | 25.0 deg C | (1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.67 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 135:280493 CA
TI Photopolymerization initiator of oxime ester for light-sensitive photoresist composition
IN Kunimoto, Kazuhiko; Oka, Hidetaka; Ohwa, Masaki; Tanabe, Junichi; Kura, Hisatoshi; Birbaum, Jean Luc
PA Ciba Specialty Chemicals Holding Inc., Switz.
SO Fr. Demande, 171 pp.
CODEN: FRXXBL
DT Patent
LA French
IC ICM C07C251-36
ICS C07C251-38; C07C251-40; C07C251-52; C07C251-54; C07C323-47; C07D333-22; G03F007-031; C08F002-50; G03C009-08
CC 74-5 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 35
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 2802528	A1	20010622	FR 2000-16306	20001214
	TW 499411	B	20020821	TW 2000-89123924	20001110
	NL 1016815	A1	20010618	NL 2000-1016815	20001206
	NL 1016815	C2	20020514		
	GB 2358017	A1	20010711	GB 2000-29793	20001207
	GB 2358017	B2	20020313		
	SE 2000004564	A	20020612	SE 2000-4564	20001211
	SE 522774	C2	20040302		
	US 2001012596	A1	20010809	US 2000-734625	20001212
	JP 2001233842	A2	20010828	JP 2000-377671	20001212
	IT 1319688	B1	20031023	IT 2000-MI2676	20001212
	CA 2328376	AA	20010615	CA 2000-2328376	20001213
	FI 2000002730	A	20010616	FI 2000-2730	20001213
	DE 10061947	A1	20010621	DE 2000-10061947	20001213
	ES 2177438	A1	20021201	ES 2000-2977	20001213
	ES 2177438	B1	20041016		
	DK 200001878	A5	20010616	DK 2000-1878	20001214
	BE 1013872	A5	20021105	BE 2000-789	20001214
	CN 1299812	A	20010620	CN 2000-135980	20001215
	BR 2000006379	A	20010724	BR 2000-6379	20001215
PRAI	EP 1999-811160	19991215			
	EP 2000-810629	20000717			

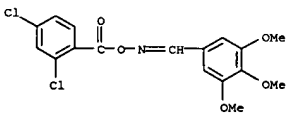
AB The invention relates to a photopolymn. initiator of oxime ester for a photoresist composition, wherein the oxime is derivative of Ar1-C=N-OR1(H) (R1 =

L6 ANSWER 53 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)
cycloalkanoyl, benzoyl, alkenoyl; Ar1 = aryl, aroyl). The photopolymn. initiator provides the alkali-developable light-sensitive photoresist compn., which shows the improved storageability, of the high resoln. and the good storageability.
ST photopolymn initiator oxime ester light sensitive photoresist compn
IT Light-sensitive materials
Photoresists
(light-sensitive color filter composition containing oxime esters used in optical imaging devices)
IT Polymerization catalysts
(photopolymn.; light-sensitive color filter composition containing oxime esters used in optical imaging devices)
IT 333438-68-9P 362624-48-4P 362624-51-9P 362624-52-0P 362624-53-1P
362624-54-2P 362624-55-3P 362624-56-4P 362624-57-5P 362624-58-6P
362624-59-7P 362624-60-0P 362624-61-1P 362624-62-2P 362624-63-3P
362624-64-4P 362624-65-5P 362624-66-6P 362624-67-7P 362624-68-8P
362624-69-9P 362624-70-2P 362624-71-3P 362624-72-4P 362624-73-5P
362624-74-6P 362624-75-7P 362624-76-8P 362624-77-9P 362624-78-0P
362624-79-1P 362624-80-4P 362624-81-5P 362624-82-6P 362624-83-7P
362624-84-8P 362624-85-9P 362624-87-1P 362624-88-2P 362624-89-3P
362624-90-6P 362624-91-7P 362624-92-8P 362624-94-0P 362624-96-2P
362624-97-3P 362624-98-4P 362624-99-5P 362625-00-1P 362625-01-2P
362625-03-4P 362625-04-5P 362625-06-7P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(light-sensitive color filter composition containing oxime esters used in optical imaging devices)
IT 74-88-4, Iodomethane, reactions 75-36-5, Acetyl chloride 104-88-1, 4-Chlorobenzaldehyde, reactions 108-98-5, Benzenethiol, reactions 127-09-3, Sodium acetate 5470-11-1, Hydroxylamine, hydrochloride 38360-81-5, 3,5-Dimethylbenzenethiol
RL: RCT (Reactant); RACT (Reactant or reagent)
(light-sensitive color filter composition containing oxime esters used in optical imaging devices)
IT 1208-88-4P, Benzaldehyde, 4-(phenylthio)- 66794-11-4P 84211-99-4P 362624-49-5P 362624-50-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(light-sensitive color filter composition containing oxime esters used in optical imaging devices)

L6 ANSWER 54 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN
RN 284679-88-5 REGISTRY
ED Entered STN: 10 Aug 2000
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(2,4-dichlorobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H15 Cl2 N O5
SR CAS Client Services
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	2134	pH 1	(1) ACD
Bioconc. Factor (BCF)	2134	pH 4	(1) ACD
Bioconc. Factor (BCF)	2134	pH 7	(1) ACD
Bioconc. Factor (BCF)	2134	pH 8	(1) ACD
Bioconc. Factor (BCF)	2134	pH 10	(1) ACD
Boiling Point (BP)	509.4+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	77.99+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	261.9+/-59.2 deg C		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	8407	pH 1	(1) ACD
Koc (KOC)	8407	pH 4	(1) ACD
Koc (KOC)	8407	pH 7	(1) ACD
Koc (KOC)	8407	pH 8	(1) ACD
Koc (KOC)	8407	pH 10	(1) ACD
logD (LOGD)	4.68	pH 1	(1) ACD
logD (LOGD)	4.68	pH 4	(1) ACD
logD (LOGD)	4.68	pH 7	(1) ACD
logD (LOGD)	4.68	pH 8	(1) ACD
logD (LOGD)	4.68	pH 10	(1) ACD
logP (LOGP)	4.683+/-0.602		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

L6 ANSWER 54 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	384.21		(1) ACD
Vapor Pressure (VP)	1.70E-10 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.67 ((C) 1994-2005 ACD/Labs)

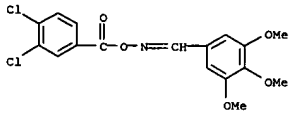
See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 55 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN

RN 284679-87-4 REGISTRY
ED Entered STN: 10 Aug 2000
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(3,4-dichlorobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H15 Cl2 N O5
SR CAS Client Services
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	4990	pH 1	(1) ACD
Bioconc. Factor (BCF)	4990	pH 4	(1) ACD
Bioconc. Factor (BCF)	4990	pH 7	(1) ACD
Bioconc. Factor (BCF)	4990	pH 8	(1) ACD
Bioconc. Factor (BCF)	4990	pH 10	(1) ACD
Boiling Point (BP)	512.6+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	78.38+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	263.8+/-59.2 deg C		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	15443	pH 1	(1) ACD
Koc (KOC)	15443	pH 4	(1) ACD
Koc (KOC)	15443	pH 7	(1) ACD
Koc (KOC)	15443	pH 8	(1) ACD
Koc (KOC)	15443	pH 10	(1) ACD
logD (LOGD)	5.17	pH 1	(1) ACD
logD (LOGD)	5.17	pH 4	(1) ACD
logD (LOGD)	5.17	pH 7	(1) ACD
logD (LOGD)	5.17	pH 8	(1) ACD
logD (LOGD)	5.17	pH 10	(1) ACD
logP (LOGP)	5.169+/-0.600		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

L6 ANSWER 55 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	384.21		(1) ACD
Vapor Pressure (VP)	1.27E-10 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.67 ((C) 1994-2005 ACD/Labs)

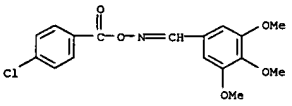
See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 56 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN

RN 284679-86-3 REGISTRY
ED Entered STN: 10 Aug 2000
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(4-chlorobenzoyl)oxime (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H16 Cl N O5
SR CAS Client Services
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1543	pH 1	(1) ACD
Bioconc. Factor (BCF)	1543	pH 4	(1) ACD
Bioconc. Factor (BCF)	1543	pH 7	(1) ACD
Bioconc. Factor (BCF)	1543	pH 8	(1) ACD
Bioconc. Factor (BCF)	1543	pH 10	(1) ACD
Boiling Point (BP)	477.4+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	74.12+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	242.5+/-56.7 deg C		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	6664	pH 1	(1) ACD
Koc (KOC)	6664	pH 4	(1) ACD
Koc (KOC)	6664	pH 7	(1) ACD
Koc (KOC)	6664	pH 8	(1) ACD
Koc (KOC)	6664	pH 10	(1) ACD
logD (LOGD)	4.50	pH 1	(1) ACD
logD (LOGD)	4.50	pH 4	(1) ACD
logD (LOGD)	4.50	pH 7	(1) ACD
logD (LOGD)	4.50	pH 8	(1) ACD
logD (LOGD)	4.50	pH 10	(1) ACD
logP (LOGP)	4.498+/-0.591		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

L6 ANSWER 56 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	349.77		(1) ACD
Vapor Pressure (VP)	2.82E-09 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.67 ((C) 1994-2005 ACD/Labs)

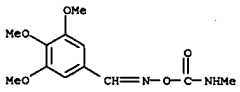
See HELP PROPERTIES for information about property data sources in REGISTRY.

L6 ANSWER 57 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN

RN 2815-72-7 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzaldehyde, 3,4,5-trimethoxy-, O-(methylcarbamoyl)oxime (7CI, 8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H16 N2 O5
LC STN Files: CA, CAOLD, CAPLUS, TOXCENTER
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: NORL (No role in record)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	13.7	pH 1	(1) ACD
Bioconc. Factor (BCF)	13.8	pH 4	(1) ACD
Bioconc. Factor (BCF)	13.8	pH 7	(1) ACD
Bioconc. Factor (BCF)	13.8	pH 8	(1) ACD
Bioconc. Factor (BCF)	13.8	pH 10	(1) ACD
Freely Rotatable Bonds (FRB)	6		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	1		(1) ACD
Koc (KOC)	226	pH 1	(1) ACD
Koc (KOC)	228	pH 4	(1) ACD
Koc (KOC)	228	pH 7	(1) ACD
Koc (KOC)	228	pH 8	(1) ACD
Koc (KOC)	228	pH 10	(1) ACD
logD (LOGD)	1.80	pH 1	(1) ACD
logD (LOGD)	1.80	pH 4	(1) ACD
logD (LOGD)	1.80	pH 7	(1) ACD
logD (LOGD)	1.80	pH 8	(1) ACD
logD (LOGD)	1.80	pH 10	(1) ACD
logP (LOGP)	1.802+/-0.588		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD

L6 ANSWER 57 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	268.27		(1) ACD
pKa (PKA)	13.72+/-0.46	Most Acidic	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1

AN 62:25221 CA
TI Influence of the methylenedioxyphenyl structure in synergism of a carbamate insecticide for house flies
AU Moorefield, Herbert H.; Weiden, Mathias H. J.
CS Union Carbide Agr. Res. Sta., Clayton, NC
SO Contributions from Boyce Thompson Institute (1964), 22(8), 425-33
CODEN: CBTIAE; ISSN: 0006-8543
DT Journal
LA English
CC 72 (Pesticides)
AB Carbaryl was applied topically, singly, and in combination with several series of adjuvants to the housefly to determine the role of the dioxole ring of methylenedioxyphenyl compds. in synergizing the carbamate insecticides.
When the methylenedioxy moiety was replaced with methoxyl or methoxyl and hydroxyl groups, synergistic activity was greatly reduced or lost. Several 1,3-benzodioxans also failed to act as synergists. The integrity of the 1,2-methylenedioxy structure is essential for maximum potentiation of housefly toxicity of the carbamates, paralleling the case for pyrethrins synergism.
IT Houseflies
(carbamate insecticide effect on, synergism of compds. containing (methylenedioxy)phenyl group for)
IT Phenol, 3,4-(methylenedioxy)-, methylcarbamate
(as synergist for carbaryl, in housefly control)
IT (Methylenedioxy)phenyl group
(synergism with carbamate insecticides of compds. containing)
IT 6414-57-9, Carbamic acid, methyl-
(3,4,5-trimethoxybenzaldehyde oxime derivative, as synergist for carbaryl, in housefly control)
IT 93-03-8, Veratryl alcohol 93-07-2, Veratric acid 93-15-2, Benzene, 4-allyl-1,2-dimethoxy- 94-59-7, Benzene, 4-allyl-1,2-(methylenedioxy)- 120-14-9, Veratraldehyde 120-57-0, Piperonal 120-60-5, Carbamic acid, methyl-, 3,4-(methylenedioxy)phenyl ester 121-33-5, Vanillin 121-34-6, Vanillic acid 274-09-9, Benzene, 1,2-(methylenedioxy)- 495-76-1, Piperonyl alcohol 533-31-3, Phenol, 3,4-(methylenedioxy)- 1135-24-6, Cinnamic acid, 4-hydroxy-3-methoxy- 2033-89-8, Phenol, 3,4-dimethoxy- 2089-36-3, Piperonal, oxime 2169-98-4, Veratraldehyde, oxime 2620-43-1, Piperonyl alcohol, methylcarbamate 2631-35-8, Piperonal,

L6 ANSWER 57 OF 57 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)
O-(methylcarbamoyl)oxime 2635-13-4, Benzene, 4-bromo-1,2-(methylenedioxy) 2815-67-0, Styrene, 2,3-dimethoxy-β-nitro- 2815-68-1, Carbamic acid, methyl-, 3,4-dimethoxyphenyl ester 2815-70-5, o-Veratraldehyde, O-(methylcarbamoyl)oxime 2815-71-6, Veratraldehyde, O-(methylcarbamoyl)oxime 2815-72-7, Benzaldehyde, 3,4,5-trimethoxy-, O-(methylcarbamoyl)oxime 2815-74-9, Veratryl alcohol, methylcarbamate 2815-74-9, Carbamic acid, methyl-, veratryl ester 2844-83-9, Acetaldehyde, 2-ethylhexyl piperonyl acetal 2859-78-1, Benzene, 4-bromo-1,2-dimethoxy- 2874-33-1, Vanillin, oxime 2878-54-8, Acetaldehyde, ethyl veratryl acetal 2878-55-9, Acetaldehyde, ethyl piperonyl acetal 2878-56-0, Acetaldehyde, 2-chloroethyl 2,3-dimethoxybenzyl acetal 2878-58-2, Acetaldehyde, 2-ethylhexyl veratryl acetal 2963-50-0, Styrene, 2,3-(methylenedioxy)-β-nitro- 28583-34-8, Acetaldehyde, 2-chloroethyl piperonyl acetal
(as synergist for carbaryl, in housefly control)
IT 91-16-7, Benzene, o-dimethoxy-
(carbaryl in relation to, in housefly control)
IT 55-38-9, Phosphorothioic acid, O,O-dimethyl O-[4-(methylthio)-m-tolyl] ester 299-84-3, Phosphorothioic acid, O,O-dimethyl O-2,4,5-trichlorophenyl ester 333-41-5, Phosphorothioic acid, O,O-diethyl O-[2-isopropyl-6-methyl-4-pyrimidinyl] ester
(housefly control by)
IT 52-68-6, Phosphonic acid, (2,2,2-trichloro-1-hydroxyethyl)-, dimethyl ester 126-22-7, Butyric acid, ester with dimethyl (2,2,2-trichloro-1-hydroxyethyl)phosphonate 919-54-0, Acetic acid, mercapto-, ethyl ester, S-ester with O,O-diethyl phosphorodithioate 2373-80-0, Cinnamic acid, 3,4-(methylenedioxy)- 2844-83-9, Toluene, α-[1-[(2-ethylhexyl)oxy]ethoxy]-3,4-(methylenedioxy)- 2859-77-0, Toluene, α-[1-(2-chloroethoxy)ethoxy]-3,4-(methylenedioxy)- 2874-31-9, Acetaldehyde, 2-chloroethyl veratryl acetal 2874-31-9, Toluene, α-[1-(2-chloroethoxy)ethoxy]-3,4-dimethoxy- 2878-53-7, Toluene, α-(1-ethoxyethoxy)-2,3-dimethoxy- 2878-53-7, Acetaldehyde, 2,3-dimethoxybenzyl Et acetal 2878-54-8, Toluene, α-(1-ethoxyethoxy)-3,4-dimethoxy- 2878-55-9, Toluene, α-(1-ethoxyethoxy)-3,4-(methylenedioxy)- 2878-56-0, Toluene, α-[1-(2-chloroethoxy)ethoxy]-2,3-dimethoxy- 2878-57-1, Toluene, α-[1-[(2-ethylhexyl)oxy]ethoxy]-2,3-dimethoxy- 2878-57-1, Acetaldehyde, 2,3-dimethoxybenzyl 2-ethylhexyl acetal 2878-58-2, Toluene, α-[1-[(2-ethylhexyl)oxy]ethoxy]-3,4-dimethoxy-
(in housefly control)
IT 63-25-2, Carbamic acid, methyl-, 1-naphthyl ester
(in housefly control, compds. containing (methylenedioxy)phenyl group as synergists for)
IT 2620-43-1, Carbamic acid, methyl-, piperonyl ester
(insecticidal activity and synergism of, as synergist for carbaryl, in housefly control)
IT 6414-57-9, Carbamic acid, methyl-
(piperonal oxime derivative, as synergist for carbaryl, in housefly control)
IT 6414-57-9, Carbamic acid, methyl-
(veratraldehyde oxime derivative, as synergist for carbaryl, in housefly control)
IT 6414-57-9, Carbamic acid, methyl-
(o-vertraldehyde oxime derivative, as synergist for carbaryl, in housefly control)

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	274.82	742.62

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.36	-5.74

FILE 'REGISTRY' ENTERED AT 15:02:34 ON 06 FEB 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 4 FEB 2005 HIGHEST RN 825667-31-0
DICTIONARY FILE UPDATES: 4 FEB 2005 HIGHEST RN 825667-31-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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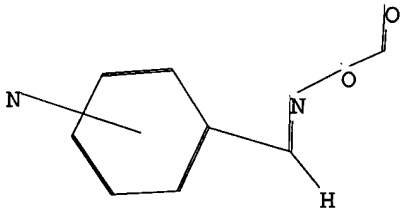
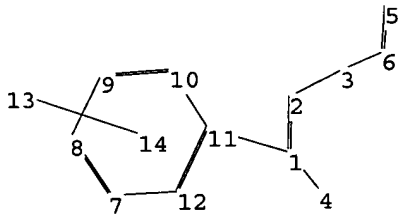
Uploading C:\Program Files\Stnexp\Queries\09734625.str





chain nodes :
1 2 3 4 5 6 13
ring nodes :
7 8 9 10 11 12
chain bonds :
1-2 1-4 1-11 2-3 3-6 5-6
ring bonds :
7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-2 2-3 3-6 5-6
exact bonds :
1-4 1-11
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12

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Match level :
1:CLASS  2:CLASS  3:CLASS  4:CLASS  5:CLASS  6:CLASS  7:Atom  8:Atom  9:Atom
10:Atom  11:Atom  12:Atom  13:CLASS  14:CLASS      .


L9      STRUCTURE UPLOADED

=> d query
L9              STR
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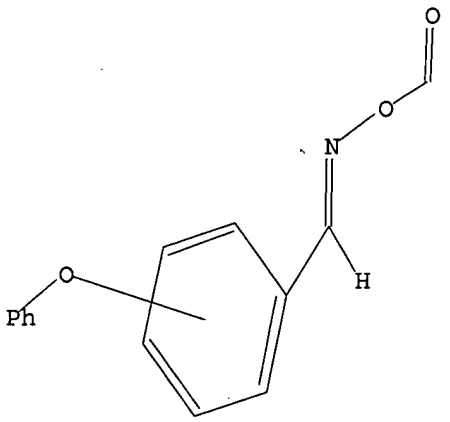


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Structure attributes must be viewed using STN Express query preparation.


=> s l9
SAMPLE SEARCH INITIATED 15:04:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    373 TO ITERATE

100.0% PROCESSED     373 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          6302 TO     8618
PROJECTED ANSWERS:                0 TO        0

L10           0 SEA SSS SAM L9

=> s l9 full
FULL SEARCH INITIATED 15:04:06 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   7152 TO ITERATE

100.0% PROCESSED    7152 ITERATIONS                             16 ANSWERS
SEARCH TIME: 00.00.01

L11          16 SEA SSS FUL L9

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COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             162.19     904.81
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-5.74

FILE 'CAPLUS' ENTERED AT 15:04:11 ON 06 FEB 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

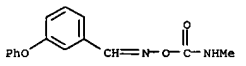
FILE COVERS 1907 - 6 Feb 2005 VOL 142 ISS 7
FILE LAST UPDATED: 4 Feb 2005 (20050204/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

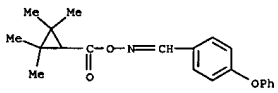
=> s l11
L12 15 L11

=> d l12 1-15 abs ibib hitstr

L12 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
AB α-X-3-phenoxybenzaldehyde O-(methylcarbamoyl) oximes (X = H, cyano, or ethylthio) were synthesized by condensation of 3-phenoxybenzaldehyde with hydroxylamine, chlorination, substitution reaction with MX, and Curtis reaction with acetyl hydrazide, and characterized by IR, 1H-NMR, and elemental anal. Their insecticidal activity was studied. The exptl. results of insecticidal activity showed that these compds. had the notable
effect on the Aphis medicaginis Koch.
ACCESSION NUMBER: 2002:866345 CAPLUS
DOCUMENT NUMBER: 139:129377
TITLE: Synthesis and insecticidal activity of α-substituted benzaldehyde O-(methylcarbamoyl) oxime
AUTHOR(S): Pan, Zhongwen
CORPORATE SOURCE: Department of Pesticide, Anhui Research Institute of Chemical Industry, Hefei, 230041, Peop. Rep. China
SOURCE: Huaxue Yanjiu Yu Yingyong (2002), 14(2), 235-236
CODEN: HYYIFM; ISSN: 1004-1656
PUBLISHER: Huaxue Yanjiu Yu Yingyong Bianjibu
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 139:129377
IT **85879-19-2P**
RL: AGR (Agricultural use); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and insecticidal activity of α-substituted benzaldehyde O-(methylcarbamoyl) oxime)
RN 85879-19-2 CAPLUS
CN Benzaldehyde, 3-phenoxy-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)

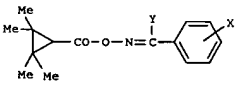


L12 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
AB A series of compds. containing oxime-ester linkage in place of the ester linkage in pyrethroid ester were designed and prepared Bioassay data of insecticidal activities of these compds. on Ostrinia nubilalis (H.) and Culex pipiens (L.) are presented. Among them 4-dimethyaminobenzaldehyde oxime ester of 2,2,3,3-tetramethylcyclopropanecarboxylic acid and 4-dimethyamino benzaldehyde oxime ester of cyclopropanecarboxylic acid were found to be potent insecticide against Ostrinia nubilalis (H.). Structure-activity relationship of the compds. is discussed.
ACCESSION NUMBER: 2002:310814 CAPLUS
DOCUMENT NUMBER: 137:121038
TITLE: Synthesis and insecticidal activities of new pyrethroid acid oxime ester derivatives
AUTHOR(S): Ma, Jun'an; Huang, Runqiu; Chai, Youxin
CORPORATE SOURCE: Institute and State Key Laboratory of Elemento-organic
Chemistry, Nankai University, Tianjin, 300071, Peop. Rep. China
SOURCE: Progress in Natural Science (2002), 12(4), 271-277
CODEN: PNASEA; ISSN: 1002-0071
PUBLISHER: Science in China Press
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:121038
IT **246532-28-5P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and insecticidal activities of)
RN 246532-28-5 CAPLUS
CN Benzaldehyde, 4-phenoxy-, O-[(2,2,3,3-tetramethylcyclopropyl)carbonyl]oxime (9CI) (CA INDEX NAME)



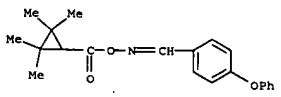
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
GI



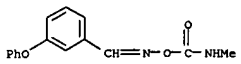
I

AB Twenty new substituted benzaldehyde oxime tetramethylcyclopropane carboxylates I (X = H, 4-C6H5OC6H4, 4-CH3, 4-(CH3)2CH, 4-(CH3)3C, 4-Cl, 4-NO2, 4-NM2, 2-Cl-4-NMe2, 3,5-Cl2NMe2; Y = H, Cl, CN; etc.) were prepared
and tested as pesticides. The preliminary bioassays indicated that compds. I (X = 4-Me2N, 4-Et2N; Y = H) showed high insecticidal activity.
ACCESSION NUMBER: 1999:532271 CAPLUS
DOCUMENT NUMBER: 131:286241
TITLE: Synthesis and bioactivity of substituted benzaldehyde oxime carboxylates. (III) - Synthesis and bioactivity of substituted benzaldehyde oxime tetramethylcyclopropanecarboxylates
AUTHOR(S): Ma, Jun-An; Huang, Run-Qiu; Chai, You-Xin
CORPORATE SOURCE: Inst. State Key Elemento-organic Chemistry, Nankai Univ., Tianjin, 300071, Peop. Rep. China
SOURCE: Gaodeng Xuexiao Huaxue Xuebao (1999), 20(5), 747-749
CODEN: KTHPDM; ISSN: 0251-0790
PUBLISHER: Gaodeng Jiaoyu Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
IT **246532-28-5P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of O-tetramethylcyclopropanecarbonyl benzoyloximes as pesticides)
RN 246532-28-5 CAPLUS
CN Benzaldehyde, 4-phenoxy-, O-[(2,2,3,3-tetramethylcyclopropyl)carbonyl]oxime (9CI) (CA INDEX NAME)



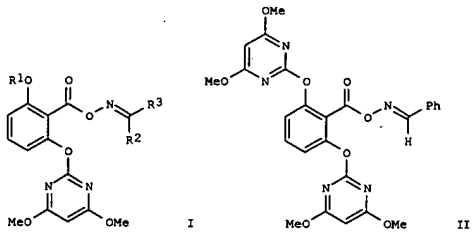
L12 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
AB A bioconcn. ratio (BCR) represents the ratio of the concentration of a chemical in
an exposed biol. system, such as a plant or fish, to the concentration in the
exposure medium (water, soil, air). A comparison was made of the precision and accuracy of the mol. connectivity index (MCI) and the octanol/water partition coefficient (Kow) as predictors of BCR from the soil
matrix into above- or below-ground vegetation tissues. Calculated octanol/air
partition coefficient (Koa) values were compared with calculated Kow and MCI values
as predictors of measured air-to-plant BCR. Based on a statistical evaluation of explained variance, residual error, and cross-validation, this evaluation showed that the MCI provides higher precision, greater ease of use, and a more cost-effective method to predict the potential bioconcn. of a chemical from soil into above-ground vegetation. Statistical
analyses of the various methods showed that the Kow and MCI approaches have a similar level of precision for predicting BCR from soil solution into
roots and, among MCI, Koa, and Kow, Koa is somewhat more precise and valid
than MCI and Kow to estimate uptake, but all have limited accuracy as bioconcn. predictors. These latter results were derived mainly from the paucity of reliable Koa values and measured air-to-plant BCR indicated a need for more exptl. measurements from which more accurate models may be developed.
ACCESSION NUMBER: 1997:771780 CAPLUS
DOCUMENT NUMBER: 128:38697
TITLE: Predicting plant uptake of organic chemicals from soil
or air using octanol/water and octanol/air partition ratios and a molecular connectivity index
AUTHOR(S): Dowdy, Deanna L.; Mckone, Thomas E.
CORPORATE SOURCE: Department of Environmental Toxicology, Risk Sciences Program, University of California, Davis, CA, 95617-8588, USA
SOURCE: Environmental Toxicology and Chemistry (1997), 16(12),
2448-2456
CODEN: ETOCDK; ISSN: 0730-7268
PUBLISHER: SETAC Press
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **85879-19-2**
RL: BPR (Biological process); BSU (Biological study, unclassified); POL (Pollutant); REM (Removal or disposal); BIOL (Biological study); OCCU (Occurrence); PROC (Process)
(predicting bioconcn. ratio for plant uptake of organic chems. from soil
or air using octanol/water and octanol/air partition ratios and mol. connectivity index)
RN 85879-19-2 CAPLUS
CN Benzaldehyde, 3-phenoxy-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)

L12 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L12 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
GI



AB The invention relates to novel herbicidal pyrimidine derivs. I [R1 = 4,6-dimethoxy-2-pyrimidinyl, C1-4 alkyl, C2-4 alkenyl, acyl, alkylsulfonyl
or heteroarylmethyl; R2 = H, halo, cyano, NO2, C1-8 alkyl, C1-8 alkoxy, C1-8 alkythio, C1-8 alkoxycarbonyl, C2-4 alkenyloxycarbonyl, (hetero)arylmethoxycarbonyl, C1-4 alkylaminocarbonyl, aryl-C1-4 alkylaminocarbonyl, heteroarylmethylaminocarbonyl, aryl, C2-8 alkenyl, C3-6 cycloalkyl, PhCH2, aryloxy, arylthio, or C1-8 alkylcarbonyl; R3 = (un)substituted Ph, COR4; R4 = H, C1-4 alkyl, C2-4 alkenyl, C3-6 cycloalkyl, PhCH2, aryl, C1-4 alkoxy, C2-4 alkenyloxy, C3-6 cycloalkoxy, PhCH2O, aryloxy, C1-4 alkythio, C2-4 alkenylthio, C3-6 cycloalkylthio, PhCH2S, arythio, amino which can be substituted with C1-C4 alkyl or aryl or arylmethyl], as well as a process for their preparation, and their herbicidal compns. I have excellent activity against both narrow- and broadleaf weeds, with increased safety for crops (especially directly sown
rice). For example, 2,6-bis(4,6-dimethoxypyrimidin-2-yl)oxybenzoic acid was treated with 2,2'-dipyridyl disulfide and PPh3 in PhMe to give 90% of the corresponding 2-pyridyl thioester, which reacted with benzaldehyde oxime in CH2Cl2 in the presence of CuBr2 to give 85% title compound II. At
63 g/ha postemergence under paddy field conditions, II gave complete control of 7 weeds with no damage to direct-sown rice seedlings. Characterizing phys. and herbicidal data for 73 compds. are given.

ACCESSION NUMBER: 1995:810566 CAPLUS
DOCUMENT NUMBER: 123:228208
TITLE: Pyrimidine derivatives, process for their preparation,
and their use as herbicides.
INVENTOR(S): Hur, Chang Uk; Cho, Jin Ho; Hong, Su Myeong; Kim, Hong
Woo; Lim, Young Hee; Rim, Jae Suk; Kim, Jeong Su; Chae, Sang Heon
PATENT ASSIGNEE(S): Lucky Ltd., S. Korea
SOURCE: Eur. Pat. Appl., 54 pp.

L12 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

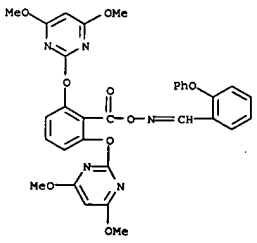
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 658549	A1	19950621	EP 1994-117857	19941111
EP 658549	B1	20010523		
R: CH, DE, FR, GB, LI, NL				
KR 9701480	B1	19970206	KR 1993-24099	19931113
KR 120271	B1	19971104	KR 1993-30055	19931227
KR 120270	B1	19971104	KR 1993-31016	19931229
US 5521146	A	19960528	US 1994-339249	19941110
BR 9404436	A	19951017	BR 1994-4436	19941111
CN 1111623	A	19951115	CN 1994-117926	19941111
CN 1043885	B	19990630		
AU 9478812	A1	19950608	AU 1994-78812	19941114
AU 673629	B2	19961114		
JP 07196629	A2	19950801	JP 1994-279506	19941114
JP 2517215	B2	19960724		

PRIORITY APPLN. INFO.:
KR 1993-24099 A 19931113
KR 1993-30055 A 19931227
KR 1993-31016 A 19931229

OTHER SOURCE(S): CASREACT 123:228208; MARPAT 123:228208

IT **168088-51-5P 168088-52-6P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidine derivs. as herbicides)

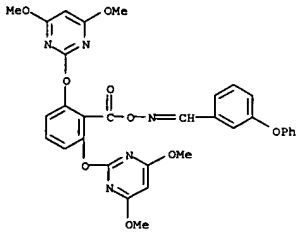
RN 168088-51-5 CAPLUS
CN Benzaldehyde, 2-phenoxy-, O-[2,6-bis[(4,6-dimethoxy-2-pyrimidinyl)oxy]benzoyl]oxime (9CI) (CA INDEX NAME)



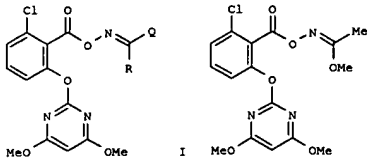
RN 168088-52-6 CAPLUS

L12 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

CN Benzaldehyde, 3-phenoxy-, O-[2,6-bis[(4,6-dimethoxy-2-pyrimidinyl)oxy]benzoyl]oxime (9CI) (CA INDEX NAME)



L12 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
GI



AB New 6-chloro-2-[(4,6-dimethoxy-2-pyrimidinyl)oxy]benzoates [[2-[[(alkyleneamino)oxy]carbonyl]-1-chloro-3-phenoxy]pyrimidines] I (R = H, halo, cyano, etc.; Q = alkyl, alkenyl, cycloalkyl, etc.) were disclosed. I were claimed as herbicides. An example compound 2-[1-chloro-[[[(1-methoxyethylidene)amino]oxy]carbonyl]phenoxy]-4,6-dimethoxypyrimidine (II) was prepared

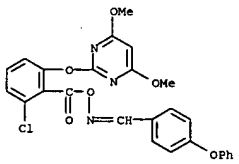
ACCESSION NUMBER: 1994:605344 CAPLUS
DOCUMENT NUMBER: 121:205344
TITLE: Novel 6-chloro-2-(4,6-dimethoxypyrimidin-2-yl) oxybenzoic acid ester derivatives, processes for their production and their application as herbicides.
INVENTOR(S): Hur, Chang Uk; Cho, Jin Ho; Lee, Ho Seong; Yoo, Sang Ku; Hong, Su Myeong; Kim, Hong Woo; Rim, Jae Suk; Bae, Yeong Tae; Chae, Sand Heon; et al.
PATENT ASSIGNEE(S): Lucky Ltd., S. Korea
SOURCE: Eur. Pat. Appl., 82 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 608862	A1	19940803	EP 1994-101132	19940126
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
KR 9603323	B1	19960308	KR 1993-1017	19930127
KR 9612180	B1	19960916	KR 1993-10097	19930604
KR 9612179	B1	19960916	KR 1993-10098	19930604
KR 9612181	B1	19960916	KR 1993-10099	19930604
KR 9612194	B1	19960916	KR 1993-10100	19930604
KR 9612195	B1	19960916	KR 1993-10101	19930604
CN 1101345	A	19950412	CN 1994-102665	19940126
US 5494888	A	19960227	US 1994-186589	19940126
BR 9400365	A	19940816	BR 1994-365	19940127
JP 07149735	A2	19950613	JP 1994-7824	19940127
JP 2543665	B2	19961016		

L12 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

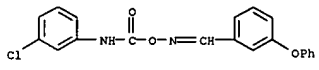
IN 182571	A	19990508	IN 1994-DE86	19940128
IN 183197	A	19991002	IN 1994-DE1445	19941111
PRIORITY APPLN. INFO.:			KR 1993-1017 A	19930127
			KR 1993-10097 A	19930604
			KR 1993-10098 A	19930604
			KR 1993-10099 A	19930604
			KR 1993-10100 A	19930604
			KR 1993-10101 A	19930604
			EP 1994-101132 A	19940126

OTHER SOURCE(S): MARPAT 121:205344
IT **157990-11-9P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide)
RN 157990-11-9 CAPLUS
CN Benzaldehyde, 4-phenoxy-, O-[2-chloro-6-[(4,6-dimethoxy-2-pyrimidinyl)oxy]benzoyl]oxime (9CI) (CA INDEX NAME)

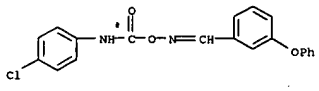


L12 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
AB The title reaction gave the corresponding carbamates or ureas. Thus, reaction of 3-PhOC6H4CH(OH)P(O)(OEt)2 with 3-ClC6H4NCO gave 90% 3-PhOC6H4CH[P(O)(OEt)2]O2CNHC6H4Cl-3.

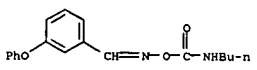
ACCESSION NUMBER: 1992:511702 CAPLUS
DOCUMENT NUMBER: 117:111702
TITLE: Reaction of O,O-dialkyl 3-phenoxy-α-hydroxy(amino)benzylphosphonates and the E isomer of 3-phenoxybenzaldoxime with isocyanates
AUTHOR(S): Abdullaev, N. B.; Galymzhanov, S. A.; Erzhanova, M. S.; Promonenkov, V. K.
CORPORATE SOURCE: Kaz. Gos. Univ., Alma-Ata, Kazakhstan
SOURCE: Izvestiya Akademii Nauk Respubliki Kazakhstan, Seriya Khimicheskaya (1992), (1), 90-4
CODEN: IARREQ
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 117:111702
IT **143057-00-5P 143057-01-6P 143057-02-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 143057-00-5 CAPLUS
CN Benzaldehyde, 3-phenoxy-, O-[[(3-chlorophenyl)amino]carbonyl]oxime (9CI) (CA INDEX NAME)



RN 143057-01-6 CAPLUS
CN Benzaldehyde, 3-phenoxy-, O-[[(4-chlorophenyl)amino]carbonyl]oxime (9CI) (CA INDEX NAME)



RN 143057-02-7 CAPLUS
CN Benzaldehyde, 3-phenoxy-, O-[(butylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



L12 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
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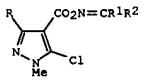
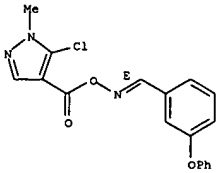


I

AB A series of novel 1,3-substituted 5-chloropyrazole-4-carboxylic acid oxime esters I (R = H, Me; R1 = H, Me, Et; R2 = Ph, Me, substituted Ph; R1R2 = cyclohexylidene) was synthesized. Their chemical structures were elucidated by 1H, 13C-NMR and IR spectra. Fifteen such compds. were screened for their antifungal activity. The results showed that pyrazole oxime esters with electron withdrawing groups had better biol. activities than those with electron releasing groups.

ACCESSION NUMBER: 1991:23855 CAPLUS
DOCUMENT NUMBER: 114:23855
TITLE: Synthesis and antifungal activity of 1,3-substituted 5-chloropyrazole-4-carboxylic acid oxime esters
AUTHOR(S): Khim, Yong Whan; Park, Chi Hyun; Choi, Weon Seok; Kwon, Young Chil; Park, Chang Kyu
CORPORATE SOURCE: OCI Res. Cent., Inchon, S. Korea
SOURCE: Han'guk Nonghwa Hakhoechi (1989), 32(4), 401-7
CODEN: JKACA7; ISSN: 0368-2897
DOCUMENT TYPE: Journal
LANGUAGE: Korean
IT **131141-98-5P 131142-03-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and fungicidal activity of)
RN 131141-98-5 CAPLUS
CN Benzaldehyde, 3-phenoxy-, O-[(5-chloro-1-methyl-1H-pyrazol-4-yl)carbonyl]oxime, (E)- (9CI) (CA INDEX NAME)

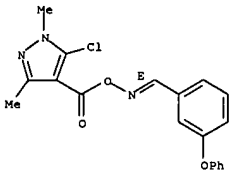
Double bond geometry as shown.



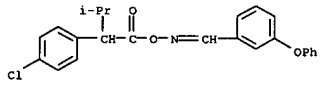
RN 131142-03-5 CAPLUS
CN Benzaldehyde, 3-phenoxy-, O-[(5-chloro-1,3-dimethyl-1H-pyrazol-4-

L12 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
yl)carbonyl]oxime, (E)- (9CI) (CA INDEX NAME)

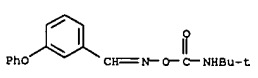
Double bond geometry as shown.



L12 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
AB A detailed examination is reported of the effect of replacement of the central
link in pyrethroids by isosteric or isoelectronic groups. The resulting change in insecticidal activity is shown to depend on the particular groups present in the other parts of the mol. A wide range (42 variations) of central groups in different combinations are synthesized and tested. Results indicate that with conventionally pyrethroidal acid and alc. fragments in the mol., some isosteric replacements are tolerated,
but most other variations are unsuccessful. Particularly interesting central groups are -COCH2- and -CH:CH-CH2-(E).
ACCESSION NUMBER: 1989:2825 CAPLUS
DOCUMENT NUMBER: 110:2825
TITLE: The pyrethrins and related compounds. Part XXXII. Replacement of the central ester link
AUTHOR(S): Elliott, Michael; Farnham, Andrew W.; Janes, Norman F.; Khambay, Bhupinder P. S.
CORPORATE SOURCE: Dep. Insectic. Fungic., AFRC Inst. Arable Crops Res., Harpenden/Hertfordshire, AL5 2JQ, UK
SOURCE: Pesticide Science (1988), 23(3), 215-30
CODEN: PSSCBG; ISSN: 0031-613X
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **89171-82-4P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and insecticidal activity of)
RN 89171-82-4 CAPLUS
CN Benzaldehyde, 3-phenoxy-, O-[2-(4-chlorophenyl)-3-methyl-1-oxobutyl]oxime (9CI) (CA INDEX NAME)



L12 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
AB Structure-activity relationships were examined for the toxicity to houseflies of pyrethroid-like carbamates, esters, and related compds. lacking a cyclopropane ring. The isosteric tert-Bu α-bromoacetate and N-tert-butylcarbamate are effective acid moieties with α-cyano-m-phenoxybenzyl, m-phenoxybenzyl, and other pyrethroid alcs. and the oxidase inhibitor piperonyl butoxide strongly synergizes the toxitity in each case. The esterase inhibitor phenylsaligenin cyclic phosphonate is generally more effective in synergizing the carboxylic esters than the carbamates. Substituent effects on the activity of 15 O-(α-cyano-m-phenoxybenzyl) N-alkylcarbamates are shown by a modified Free-Wilson method to be related to the number of branches in the
alkyl group in which α branching is favorable and β and γ branching unfavorable for the activity. O-(α-Cyano-m-phenoxybenzyl) N-[(R)α-methylbenzyl]carbamate was much more toxic than the S isomer. In a series of esters, amides, and ethers, critical features for activity are both the distance between the tert-Bu and m-phenoxyphenyl groups and the nature of the central linkage providing this distance.
ACCESSION NUMBER: 1985:608839 CAPLUS
DOCUMENT NUMBER: 103:208839
TITLE: O-(α-Cyano-m-phenoxybenzyl) N-Alkyl- and N-aralkylcarbamates and related pyrethroid-like insecticides
AUTHOR(S): Kirino, Osamu; Casida, John E.
CORPORATE SOURCE: Dep. Entomol. Sci., Univ. California, Berkeley, CA, 94720, USA
SOURCE: Journal of Agricultural and Food Chemistry (1985), 33(6), 1208-13
CODEN: JAFCAU; ISSN: 0021-8561
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **98992-39-3**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
(insecticidal activity of, structure in relation to)
RN 98992-39-3 CAPLUS
CN Benzaldehyde, 3-phenoxy-, O-[[(1,1-dimethylethyl)amino]carbonyl]oxime (9CI) (CA INDEX NAME)



L12 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
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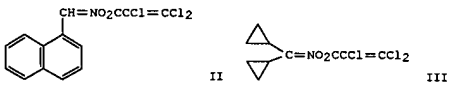
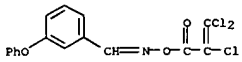


AB Cl2C:CClCO2N:CRR1 (I) (R,R1 = H, lower alkyl, benzyl, cycloalkyl, naphthyl, aryl, etc.) were prepared and shown, in some cases, to be more effective fungicides than kilazin P. Thus, 100 mL PhMe solution containing 40 g
Cl2C:CClCOCl were added at ≤20° to 30 g PhCH:NOH and 26 g Et3N in 400 mL PhMe, and the mixture was heated 2 h at 50° to give 58 g I (R = Ph, R1 = H). Among 39 other I prepared were I [R,R1 = Me,Me; Me,Et; (RR1=) cyclohexylidene), the naphthyl analog II, and the dicyclopropyl analog III.
ACCESSION NUMBER: 1984:610740 CAPLUS
DOCUMENT NUMBER: 101:210740
TITLE: Trichloroacryloyl oxime derivatives
INVENTOR(S): Yamada, Yasuo; Saito, Junichi; Gotoh, Toshio; Katsumata, Osamu; Sakawa, Shinji
PATENT ASSIGNEE(S): Nihon Tokushu Noyaku Seizo K. K. , Japan
SOURCE: Eur. Pat. Appl., 34 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

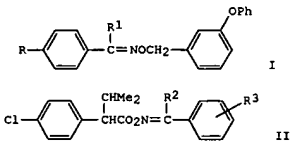
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 112524	A1	19840704	EP 1983-112276	19831207
EP 112524	B1	19860528		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL				
JP 59110665	A2	19840626	JP 1982-220165	19821217
US 4581365	A	19860408	US 1983-557688	19831202
IL 70443	A1	19870130	IL 1983-70443	19831214
BR 8306913	A	19840724	BR 1983-6913	19831215
ZA 8309329	A	19840829	ZA 1983-9329	19831215
DK 8305810	A	19840618	DK 1983-5810	19831216
AU 8322504	A1	19840621	AU 1983-22504	19831219
PRIORITY APPLN. INFO.:			JP 1982-220165 A	19821217

OTHER SOURCE(S): CASREACT 101:210740
IT **93033-15-9P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as fungicide)
RN 93033-15-9 CAPLUS
CN Benzaldehyde, 3-phenoxy-, O-(2,3,3-trichloro-1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)

L12 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L12 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
GI

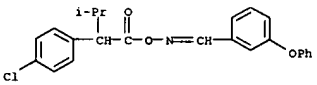


AB Title compds. I (R = F, Cl, Br, Me, Me3C, dichlorocyclopropyl, PhO; R1 = Me, Et, CHMe2, cyclopropyl) and II (R2 = H, Me, CN; R3 = H, Cl, PhO, CH2O2) were prepared E.g., stirring 4-ClC6H4C(CHMe2):NOH with 3-PhOC6H4CH2Cl in aqueous NaOH in the presence of Bu4N+ Br- gave 63% I (R = Cl, R1 = CHMe2). The latter showed high insecticidal activity against army worms and showed no inhibition of cholinesterase.

ACCESSION NUMBER: 1984:120606 CAPLUS
DOCUMENT NUMBER: 100:120606
TITLE: Oxime-ether compounds with pyrethroid-like activity
AUTHOR(S): Huang, Runqiu; Chai, Youxin; Bi, Fuchun; Chen, Xueren; Wang, Yinshu
CORPORATE SOURCE: Inst. Elem. Org. Chem., Nankai Univ., Tianjin, Peop. Rep. China
SOURCE: Gaodeng Xuexiao Huaxue Xuebao (1983), 4(5), 589-94
CODEN: KTHPDM; ISSN: 0251-0790
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

IT **89171-82-4P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and insecticidal activity of)

RN 89171-82-4 CAPLUS
CN Benzaldehyde, 3-phenoxy-, O-[2-(4-chlorophenyl)-3-methyl-1-oxobutyl]oxime (9CI) (CA INDEX NAME)



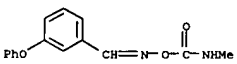
L12 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN

AB Detns. were made of the distribution of 2 series of nonionized chems., O-methylcarbamoyloximes and substituted phenylureas, in barley shoots, following uptake by the roots from solution The concns. in basal and central shoot sections became constant after 24-48 h for all but the most lipophilic chemical studied, and were then greatest for the more lipophilic chemical Amts. in the leaves generally increased up to 72 or 96 h, when degradation balanced translocation. The accumulation of chemical in the lower section of shoots can be ascribed to a partitioning process similar to that in roots, the chemical being partitioned between the shoot and the xylem transpiration stream; this uptake could be estimated from the octan-1-ol/water distribution coeffs., and was predicted to be greatest for compds. for which log Kow = 4.5.

ACCESSION NUMBER: 1984:47051 CAPLUS
DOCUMENT NUMBER: 100:47051
TITLE: Relationships between lipophilicity and the distribution of nonionized chemicals in barley shoots following uptake by the roots
AUTHOR(S): Briggs, Geoffrey; Bromilow, Richard H.; Evans, Avis A.; Williams, Mark
CORPORATE SOURCE: Rothamsted Exp. Stn., Harpenden/Hertforshire, AL5 2JQ, UK
SOURCE: Pesticide Science (1983), 14(5), 492-500
CODEN: PSSCBG; ISSN: 0031-613X
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **85879-19-2**
RL: BIOL (Biological study)
(absorption and translocation of, in barley, lipophilicity in relation to)

RN 85879-19-2 CAPLUS
CN Benzaldehyde, 3-phenoxy-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



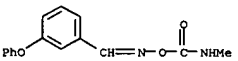
L12 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN

AB The uptake of O-methylcarbamoyloximes and substituted phenylureas by barley roots was greater the more lipophilic the chemical, and fell to a lower limiting value for polar chems. Translocation to the shoots was a passive process, and was most efficient for compds. of intermediate polarity. Both processes had reached equilibrium within 24 h of treatment. The reported behavior of many pesticides in various plant species agrees with the derived relationships, but the detailed mechanisms of these processes are unknown.

ACCESSION NUMBER: 1983:211541 CAPLUS
DOCUMENT NUMBER: 98:211541
TITLE: Relationships between lipophilicity and root uptake and translocation of nonionized chemicals by barley
AUTHOR(S): Briggs, Geoffrey; Bromilow, Richard H.; Evans, Avis A.
CORPORATE SOURCE: Rothamsted Exp. Stn., Harpenden, AL5 2JQ, UK
SOURCE: Pesticide Science (1982), 13(5), 495-504
CODEN: PSSCBG; ISSN: 0031-613X
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **85879-19-2**
RL: BIOL (Biological study)
(root uptake and translocation of, lipophilicity in relation to)

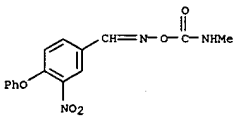
RN 85879-19-2 CAPLUS
CN Benzaldehyde, 3-phenoxy-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



L12 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
GI For diagram(s), see printed CA Issue.
AB Diphenyl ether derivs. (I; R = lower alkyl; R1 to R4 = H, halo, lower alkyl, lower alkoxy; n = 0-1; a, b = 0-1; a + b = 1-2) were prepared by reaction of II with RNCO or RNHCOCl. I had insecticidal, anticarcinogenic, and antibacterial activities. Thus, 6.0 g MeNCO and trace Et3N were added to 30.0 g p-(2-nitro-4-chlorophenoxy)benzaldehyde in THF and the mixture refluxed 1 hr to give 27.5 g O-methylcarbamoyl-p-(2-nitro-4-chlorophenoxy)benzaldoxime. Among 13 more I prepared were O-methylcarbamoyl-3-nitro-4-(m-tolyloxy)-, O-methylcarbamoyl-3-nitro-4-(p-methoxyphenoxy)-, O-methylcarbamoyl-3-nitro-4-phenoxy-, and O-methylcarbamoyl-3-nitro-4-(o-chlorophenoxy)benzaldoximes.
ACCESSION NUMBER: 1975:458415 CAPLUS
DOCUMENT NUMBER: 83:58415
TITLE: Diphenyl ether derivatives
INVENTOR(S): Kotani, Akeshi; Inamasu, Shuji
PATENT ASSIGNEE(S): Yoshitomi Pharmaceutical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 50012047	A2	19750207	JP 1973-62203	19730601
PRIORITY APPLN. INFO.:			JP 1973-62203 A	19730601

IT **56135-53-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 56135-53-6 CAPLUS
CN Benzaldehyde, 3-nitro-4-phenoxy-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



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COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 77.70 | 982.51

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION
CA SUBSCRIBER PRICE | -10.95 | -16.69

FILE 'REGISTRY' ENTERED AT 15:08:45 ON 06 FEB 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 4 FEB 2005 HIGHEST RN 825667-31-0
DICTIONARY FILE UPDATES: 4 FEB 2005 HIGHEST RN 825667-31-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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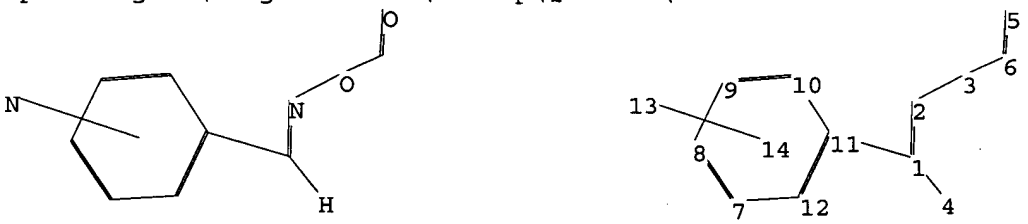

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1 2 3 4 5 6 13
ring nodes :
7 8 9 10 11 12
chain bonds :
1-2 1-4 1-11 2-3 3-6 5-6
ring bonds :
7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-2 2-3 3-6 5-6
exact bonds :
1-4 1-11
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS

L13 - STRUCTURE UPLOADED

=> d query
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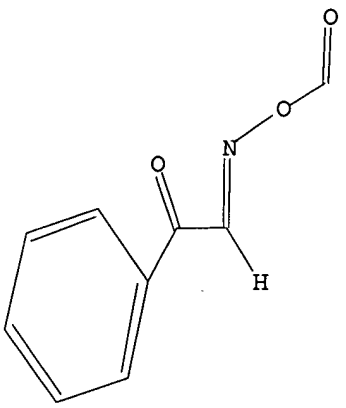

Structure attributes must be viewed using STN Express query preparation.

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FULL SEARCH INITIATED 15:13:08 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 745 TO ITERATE

100.0% PROCESSED 745 ITERATIONS 13 ANSWERS
SEARCH TIME: 00.00.01

L14 13 SEA SSS FUL L13

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	164.34	1146.85

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-16.69

FILE 'CAPLUS' ENTERED AT 15:13:17 ON 06 FEB 2005

FILE COVERS 1907 - 6 Feb 2005 VOL 142 ISS 7
FILE LAST UPDATED: 4 Feb 2005 (20050204/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l14
L15 7 L14

=> d l15 1-7 abs ibib hitstr

L15 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

AB Ketoxime-esters which generate radicals upon UV and/or visible radiation can be used in specific imaging applications and in electronics. The photogenerated radicals initiate radical polymerization of the photoimaging compns. The ketoxime-esters initiators can be used alone or in combination with sensitizers. The photosensitive compns. contg,. these initiators can be used for (1) manufacture of spacers for liquid crystal displays; (2) producing lens arrays (microlens arrays) and prism sheets for solid-state image sensors; (3) producing dielec. insulating layers in liquid crystal displays.

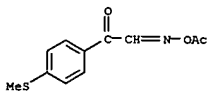
ACCESSION NUMBER: 2000:713730 CAPLUS
DOCUMENT NUMBER: 134:78558
TITLE: Use of ketoxime-esters
AUTHOR(S): Anon.
CORPORATE SOURCE: UK
SOURCE: Research Disclosure (2000), 437(Sept.), P1572-P1573 (No. 437035)
CODEN: RSDSBB; ISSN: 0374-4353
PUBLISHER: Kenneth Mason Publications Ltd.
DOCUMENT TYPE: Journal; Patent
LANGUAGE: English
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
RD 437035		20000910		
PRIORITY APPLN. INFO.:			RD 2000-437035	20000910

OTHER SOURCE(S): MARPAT 134:78558

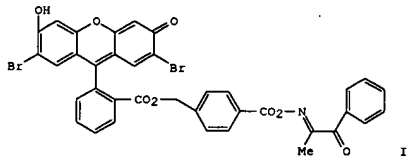
IT **314745-04-5**
RL: CAT (Catalyst use); TEM (Technical or engineered material use); USES (Uses)
(ketoxime-esters photogenerating radicals upon UV and/or visible radiation for use in photopolymg. compns. for imaging applications and in electronics)

RN 314745-04-5 CAPLUS
CN Benzeneacetaldehyde, 4-(methylthio)-α-oxo-, aldehydo-(O-acetyloxime) (9CI) (CA INDEX NAME)



L15 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

GI



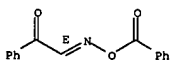
AB A new dye I which incorporated both the eosin and the O-benzoyl-α-oxooxime chromophores was synthesized and its behavior for the polymerization of 2-hydroxytethyl methacrylate (II) in the presence of a molar excess of N-methyldiethanolamine (III) was studied by differential scanning photocalorimetry. Under visible light (525 nm), I gives a greater polymerization rate than Eosin (IV) alone or a 1:1 M mixture of IV and 1-phenyl-2-(O-benzoyloxoimino)-1-propanone. A photopolymerizable mixture of I, II, III, and ethylene glycol dimethacrylate as the crosslinking monomer was evaluated as a photosensitive recording material for holog.

ACCESSION NUMBER: 1994:606082 CAPLUS
DOCUMENT NUMBER: 121:206082
TITLE: Synthesis and Evaluation as a Visible-Light Polymerization Photoinitiator of a New Eosin Ester with an O-Benzoyl-α-oxooxime Group
AUTHOR(S): Mallavia, R.; Amat-Guerri, F.; Fimia, A.; Sastre, R.
CORPORATE SOURCE: Instituto de Quimica Organica, CSIC, Madrid, 28006, Spain
SOURCE: Macromolecules (1994), 27(9), 2643-6
CODEN: MAMOBX; ISSN: 0024-9297
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **154584-15-3P 154584-16-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation with eosin)

RN 154584-15-3 CAPLUS
CN Benzeneacetaldehyde, α-oxo-, aldehydo-(O-benzoyloxime), (E)- (9CI) (CA INDEX NAME)

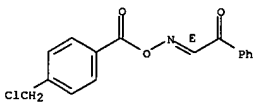
Double bond geometry as shown.



RN 154584-16-4 CAPLUS
CN Benzeneacetaldehyde, α-oxo-, aldehydo-[O-[4-(chloromethyl)benzoyl]oxime], (E)- (9CI) (CA INDEX NAME)

L15 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

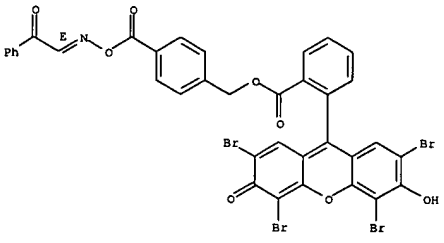
Double bond geometry as shown.



IT **154584-14-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as photoinitiators for methacrylates)

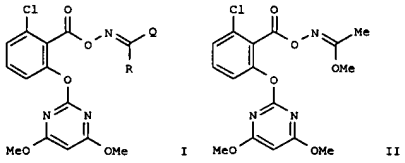
RN 154584-14-2 CAPLUS
CN Benzoic acid, 2-(2,4,5,7-tetrabromo-6-hydroxy-3-oxo-3H-xanthen-9-yl)-, [4-[[[(2-oxo-2-phenylethylidene)amino]oxy]carbonyl]phenyl]methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L15 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

GI



AB New 6-chloro-2-[(4,6-dimethoxy-2-pyrimidinyl)oxy]benzoates [[2-[[(alkyleneamino)oxy]carbonyl]-1-chloro-3-phenoxy]pyrimidines] I (R = H, halo, cyano, etc.; Q = alkyl, alkenyl, cycloalkyl, etc.) were disclosed. I were claimed as herbicides. An example compound 2-[1-chloro-[[[(1-methoxyethylidene)amino]oxy]carbonyl]phenoxy]-4,6-dimethoxypyrimidine (II) was prepared

ACCESSION NUMBER: 1994:605344 CAPLUS
DOCUMENT NUMBER: 121:205344
TITLE: Novel 6-chloro-2-(4,6-dimethoxypyrimidin-2-yl) oxybenzoic acid ester derivatives, processes for their production and their application as herbicides.
INVENTOR(S): Hur, Chang Uk; Cho, Jin Ho; Lee, Ho Seong; Yoo, Sang Ku; Hong, Su Myeong; Kim, Hong Woo; Rim, Jae Suk; Bae, Yeong Tae; Chae, Sand Heon; et al.
PATENT ASSIGNEE(S): Lucky Ltd., S. Korea
SOURCE: Eur. Pat. Appl., 82 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

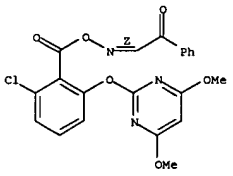
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 608862	A1	19940803	EP 1994-101132	19940126
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
KR 9603323	B1	19960308	KR 1993-1017	19930127
KR 9612180	B1	19960916	KR 1993-10097	19930604
KR 9612179	B1	19960916	KR 1993-10098	19930604
KR 9612181	B1	19960916	KR 1993-10099	19930604
KR 9612194	B1	19960916	KR 1993-10100	19930604
KR 9612195	B1	19960916	KR 1993-10101	19930604
CN 1101345	A	19950412	CN 1994-102665	19940126
US 5494888	A	19960227	US 1994-186589	19940126
BR 9400365	A	19940816	BR 1994-365	19940127
JP 07149735	A2	19950613	JP 1994-7824	19940127
JP 2543665	B2	19961016		

L15 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

IN 182571	A	19990508	IN 1994-DE86		19940128
IN 183197	A	19991002	IN 1994-DE1445		19941111
PRIORITY APPLN. INFO.:			KR 1993-1017	A	19930127
			KR 1993-10097	A	19930604
			KR 1993-10098	A	19930604
			KR 1993-10099	A	19930604
			KR 1993-10100	A	19930604
			KR 1993-10101	A	19930604
			EP 1994-101132	A	19940126

OTHER SOURCE(S): MARPAT 121:205344
IT **157991-16-7P 157991-21-4P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide)
RN 157991-16-7 CAPLUS
CN Benzeneacetaldehyde, α-oxo-, aldehydo-[O-[2-chloro-6-[(4,6-dimethoxy-2-pyrimidinyl)oxy]benzoyl]oxime], (Z)- (9CI) (CA INDEX NAME)

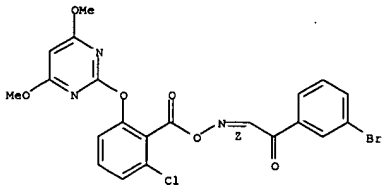
Double bond geometry as shown.



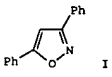
RN 157991-21-4 CAPLUS
CN Benzeneacetaldehyde, 3-bromo-α-oxo-, aldehydo-[O-[2-chloro-6-[(4,6-dimethoxy-2-pyrimidinyl)oxy]benzoyl]oxime], (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L15 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

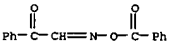


L15 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
GI



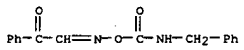
I

AB The ozonolysis of substituted isoxazoles, e.g. I, was investigated. The ozonolysis rates and the products were dependent on the site of the substituent group on isoxazole ring. The reaction mechanism of the ozonolysis of isoxazoles was also proposed.
ACCESSION NUMBER: 1994:507759 CAPLUS
DOCUMENT NUMBER: 121:107759
TITLE: Ozonolysis of substituted isoxazoles
AUTHOR(S): Kashima, Choji; Takahashi, Katsumi; Hosomi, Akira
CORPORATE SOURCE: Dep. Chem., Univ. Tsukuba, Tsukuba, 305, Japan
SOURCE: Heterocycles (1994), 37(2), 1075-82
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **24561-42-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24561-42-0 CAPLUS
CN Benzeneacetaldehyde, α-oxo-, aldehydo-(O-benzoyloxime) (9CI) (CA INDEX NAME)



L15 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
AB Among 14 potential substrates, neuropathy target esterase (NTE) hydrolyzed
Ph phenoxyacetate and Ph thiophenoxyacetate faster (1.5-1.7+) than Ph valerate, but selectivity of these substrates for NTE among the paraoxon-resistant esterases was only 35-52%. Seventy-seven other potential inhibitors (organophosphates, phosphonates, phosphoramidates, phosphinates, and carbamates) were examined to determine I50NTE and effects on
both NTE and non-NTE at 3-4 + I50NTE (I85-95) and, where possible, at 6-20 + I50NTE. Hydrophobic inhibitors with small/flexible leaving groups were generally very inhibitory: several 2,2-dichlorovinyl phosphates and fluorides were active at low nanomolar concns. In the dichlorovinyl phosphate series, increasing dialkyl chain length beyond n-pentyl decreased inhibitory power, presumably due to steric hindrance since the methyl/n-decyl ester was 15-fold more active than di-n-decyl. Chloro-substitution of both ortho-positions of a Ph leaving group for benzylcarbamates reduced inhibitory power more than 20-fold but had little
effect in a Ph leaving group of Me phenylphosphonates where the acyl-leaving group bond is longer and less subject to steric hindrance. N-Phenylbenzohydroxamyl benzylcarbamate is 10-fold more potent than any previously described carbamate against NTE. Among stereo-isomers, differences of activity ranged from <2 to 15-fold. Only diphenylphosphinyl fluoride appeared to be virtually specific for NTE: at 0.5-1 μM, it inhibited .apprx.92% of NTE and 10-13% of non-NTE which is similar to the specificity found for 2,6-dichlorophenyl Me phenylphosphonate which has been claimed to be specific. Diphenylphosphinyl fluoride has an advantage in that it is easily synthesized and should be protective rather than neuropathic, but it is not stable in store. According to first-order kinetics, concns. of inhibitor >6 + I50 should inhibit NTE >98% and for 19 out of 26 compds. a residue (2nd isoenzyme) >3% (limit of precision) was found under
these conditions: in nearly every case, the quantity was 3-5%. This quantity may not be true NTE but it cannot be the target for organophosphate-induced delayed neuropathy since it is resistant to various neuropathic and protective compds. The error of including this non-NTE in assays using the standard protocol is negligible.
ACCESSION NUMBER: 1989:130136 CAPLUS
DOCUMENT NUMBER: 110:130136
TITLE: Sensitivity and selectivity of compounds interacting with neuropathy target esterase. Further structure-activity studies
AUTHOR(S): Johnson, Martin K.
CORPORATE SOURCE: Toxicol. Unit, Med. Res. Counc. Lab., Carshalton/Surrey, SM5 4EF, UK
SOURCE: Biochemical Pharmacology (1988), 37(21), 4095-104
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **118855-72-4**
RL: BIOL (Biological study)
(neuropathy target esterase inhibition by, structure in relation to)
RN 118855-72-4 CAPLUS
CN Benzeneacetaldehyde, α-oxo-, aldehydo-[O-[[(phenylmethyl)amino]carbonyl]oxime] (9CI) (CA INDEX NAME)

L15 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



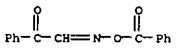
L15 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

AB O-Acylated oximinoketones RCOCR':NO2CR'' (I) were synthesized from the corresponding α,β-diketones and their structures ascertained by microanal. and NMR spectroscopy. The free radicals produced during the photolysis of I initiate the polymerization of acryl derivs. The kinetics of the photopolymns. of acrylamide and Me methacrylate were studied by gravimetric, thermometric, and dilatometric methods. The photopolymn. rate is proportional to the 1.5 power of the monomer concentration A square root dependence of the rate of photopolymn. was observed with respect to the light intensity for acrylamide, and with respect to the initiator concentration for Me methacrylate. Copolymn. of 1-phenyl-1,2-propanedione 2-O-methacryloyl oxime with Me methacrylate and polycondensation of 1-(4-hydroxyphenyl)-1,2-propanedione 2-oxime or p-hydroxyphenylglyoxal aldoxime and 2,2-bis-(4-hydroxylphenyl)propane with isophthaloyl, terephthaloyl, and sebacoyl chlorides were successful. Irradiation of these polymers produces intensive photodegradation; in the presence of monomers such as acrylamide, styrene or acrylonitrile, graft and block polymers are obtained.

ACCESSION NUMBER: 1970:477691 CAPLUS
DOCUMENT NUMBER: 73:77691
TITLE: Photopolymerization initiated by O-acyloximes
AUTHOR(S): Delzenne, Gerard A.; Laridon, Urbain L.; Peeters, H.
CORPORATE SOURCE: Photochem. Res. Lab., Gevaert-Agfa N. V., Mortsel-Antwerp, Belg.
SOURCE: European Polymer Journal (1970), 6(7), 933-43
CODEN: EUPJAG; ISSN: 0014-3057
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **24561-42-0**
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for polymerization of vinyl compds.)

RN 24561-42-0 CAPLUS
CN Benzeneacetaldehyde, α-oxo-, aldehydo-(O-benzoyloxime) (9CI) (CA INDEX NAME)



L15 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

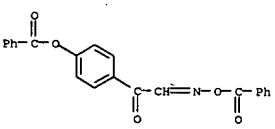
AB Photopolymerizable, ethylenically unsatd. monomers are polymerized by irradiating a mixture of the desired monomer and an O-acyl oxime initiator. Thus, various amts. of Me methacrylate (I) were dissolved in 10-3M PhCOCMe:NOBz in benzene. The solns. were sealed in tubes under N and irradiated for 120 min. with a Hg vapor lamp. The polymer was then precipitated by pouring the solution into an excess of MeOH, separated and dried (I concentration in moles/l. and mg. polymer yield given): 2.34, 300; 3.74, 762; 4.68, 1101; 5.62, 1424; 7.02, 1908; 8.42, 2238. Styrene, acrylonitrile, and acrylamide were also polymerized by this method, using as initiators MeCOCH:NOBz, MeCOCOCMe:NO2CCMe:CH2 (II), MeCOCMe:NO2CCH:CHPh, biacetyl O-(1-naphthoyl)monooxime, MeCOCMe:NOBz, biacetyl O-(o-chlorobenzoyl)monooxime, biacetyl O-(m-nitrobenzoyl)monooxime, biacetyl O-(m-methoxybenzoyl)monooxime, MeCOCPh:NOBz, PhCH:NOBz, 1-phenyl-1,2-propanedione 2-[O-(m-chlorobenzoyl)oxime], 1-phenyl-1,2-propanedione 2-[O-(p-azidobenzoyl)oxime], 1-phenyl-1,2-propanedione 2-[O-(1-anthraquinonylcarbonyl)oxime], PhCOCPh:NOBz, benzil O-(o-chlorobenzoyl)monooxime, PhCOCMe:NO2CCH2Ph, PhCOCMe:-NO2CCH:CHPh, 1-[p-(benzoyloxy)phenyl]glyoxal 2-(O-benzoyl)-oxime, 1-[p-(methacryloyloxy)phenyl]1,2-propanedione 2-(O-methacryloyl)oxime, PhCH:CHCOCH:NOBz, phenanthrenequinone (O-benzoyl)monooxime, 2,3-dihydroindene-1,2-dione 2-(O-benzoyl)oxime, O,O'-isophthaloylbis(biacetyl monooxime), and Ph-COC(SO2Ph):NOBz. I and II were copolymd., and a 1-g. portion of this copolymer and 5 ml. styrene were diluted to 20 ml. with benzene and irradiated under N giving a mixture of polystyrene, 2 different graft copolymers, and the I-II copolymer. This copolymer was used as an initiator for a variety of monomers, including (diethylamino)ethyl methacrylate. In another type of example, 1-(p-hydroxyphenyl)-1,2-propanedione 2-oxime was polycondensed with isophthaloyl dichloride, terephthaloyl dichloride, and 2,2-bis(4-hydroxyphenyl)propane, giving a copolyester, which was used as a polymerization initiator for I, giving I homopolymer and a block copolymer. A similar condensate from 1-(p-hydroxyphenyl)glyoxal 2-oxime was also used as an initiator. A mixture of 10 g. ethylene-maleic anhydride copolymer, 5 ml. triethylene glycol diacrylate, 25 mg. 2,6-di-tert-butyl-p-cresol, 50 ml. acetone, and 100 mg. PhCOCMe:NOBz was coated on a glass plate and dried to a 0.3-mm. layer. This layer was exposed 5 min. through a line neg. with a Hg lamp, and then washed with acetone, giving a very sharp relief image.

ACCESSION NUMBER: 1969:439636 CAPLUS
DOCUMENT NUMBER: 71:39636
TITLE: Unsaturated ethylenic compound photopolymers
INVENTOR(S): Laridon, Urbain L.; Delzenne, Gerard A.
PATENT ASSIGNEE(S): Gevaert-Agfa N. V.
SOURCE: Belg., 27 pp.
CODEN: BEXXAL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

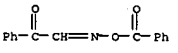
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 719039		19690205		
DE 1795089			DE	
GB 1180845			GB	
GB 1180846			GB	
US 3558309		19710000	US	
PRIORITY APPLN. INFO.:			GB	19670808

IT **22603-43-6 24561-42-0**
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for polymerization of vinyl compds. by light)

RN 22603-43-6 CAPLUS
CN Glyoxal, (p-hydroxyphenyl)-, 2-(O-benzoyloxime), benzoate (ester) (8CI) (CA INDEX NAME)



RN 24561-42-0 CAPLUS
CN Benzeneacetaldehyde, α-oxo-, aldehydo-(O-benzoyloxime) (9CI) (CA INDEX NAME)



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FULL ESTIMATED COST                                    38.63    1185.48

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CA SUBSCRIBER PRICE                                    -5.11     -21.80

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STRUCTURE FILE UPDATES:     4 FEB 2005  HIGHEST RN 825667-31-0
DICTIONARY FILE UPDATES:    4 FEB 2005  HIGHEST RN 825667-31-0

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Experimental and calculated property data are now available. For more
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http://www.cas.org/ONLINE/DBSS/registryss.html

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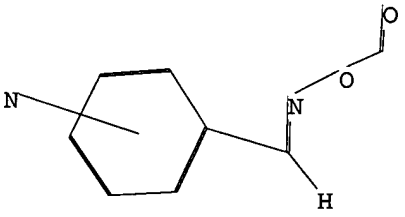

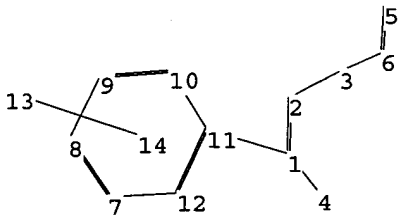


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ring nodes :
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chain bonds :
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ring bonds :
7-8  7-12  8-9  9-10  10-11  11-12
exact/norm bonds :
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exact bonds :
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normalized bonds :
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Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom
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L16 STRUCTURE UPLOADED

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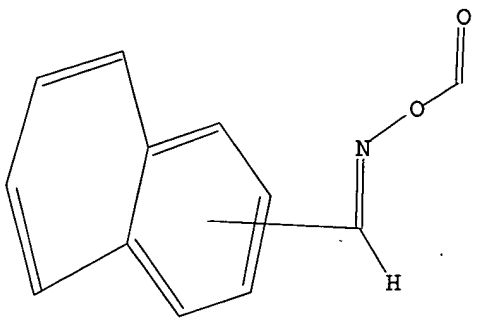

Structure attributes must be viewed using STN Express query preparation.

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SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1081 TO 2159
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L17 5 SEA SSS SAM L16

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L18 151 SEA SSS FUL L16

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FULL ESTIMATED COST	165.20	1350.68

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-21.80

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FILE COVERS 1907 - 6 Feb 2005 VOL 142 ISS 7
FILE LAST UPDATED: 4 Feb 2005 (20050204/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l18
L19 37 L18

=> d l19 1-37 abs ibib hitstr

L19 ANSWER 1 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

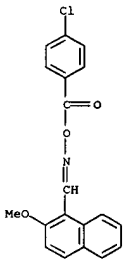
AB The title printing plate master contains a photothermal conversion material, a phenolic alkaline-soluble resin, and an organic acid precursor having a structure of -CH:NOCO- or -CONHOCO-. The printing plate master shows improved stability.

ACCESSION NUMBER: 2004:37360 CAPLUS
DOCUMENT NUMBER: 140:84686
TITLE: Positive-working offset printing plate master suitable for IR laser digital direct platemaking
INVENTOR(S): Endo, Akihiro
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 27 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004012978	A2	20040115	JP 2002-168556	20020610
PRIORITY APPLN. INFO.:			JP 2002-168556	20020610

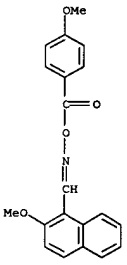
IT **99806-93-6 100906-55-6 640285-77-4 640285-78-5 640285-79-6**
RL: MOA (Modifier or additive use); USES (Uses)
(organic acid precursor; pos.-working offset printing plate master containing organic acid precursor suitable for IR laser digital direct platemaking)

RN 99806-93-6 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-(4-chlorobenzoyl)oxime (9CI) (CA INDEX NAME)

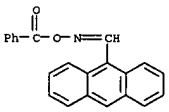


RN 100906-55-6 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-(2-naphthalenylcarbonyl)oxime (9CI) (CA INDEX NAME)

L19 ANSWER 1 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

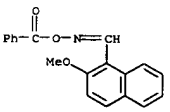


RN 640285-79-6 CAPLUS
CN 9-Anthracenecarboxaldehyde, O-benzoyloxime (9CI) (CA INDEX NAME)

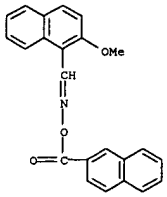


IT **99806-90-3P**
RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(organic acid precursor; pos.-working offset printing plate master containing organic acid precursor suitable for IR laser digital direct platemaking)

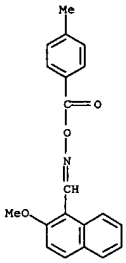
RN 99806-90-3 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-benzoyloxime (9CI) (CA INDEX NAME)



L19 ANSWER 1 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 640285-77-4 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-(4-methylbenzoyl)oxime (9CI) (CA INDEX NAME)



RN 640285-78-5 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-(4-methoxybenzoyl)oxime (9CI) (CA INDEX NAME)

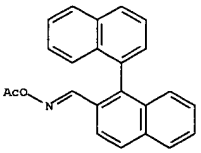
L19 ANSWER 2 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

AB Lipase-catalyzed acylation of 2-hydroxyiminomethyl-1,1'-binaphthyl and hydrolysis of 2-acetoxyiminomethyl-1,1'-binaphthyl yielded corresponding optically active oximes with high enantiomeric excess. Successful synthesis of the optically active aldehyde from its corresponding chiral O-acetyl oxime occurred without a decrease of enantiomeric excess.

ACCESSION NUMBER: 2003:807855 CAPLUS
DOCUMENT NUMBER: 140:16553
TITLE: Facile synthesis of chiral 2-formyl-1,1'-binaphthyl via lipase-catalyzed acylation and hydrolysis of 1,1'-binaphthyl oximes
AUTHOR(S): Aoyagi, Naoto; Ohwada, Tomoyuki; Izumi, Taeko
CORPORATE SOURCE: Graduate School of Science and Engineering, Department of Chemistry and Chemical Engineering, Yamagata University, Yamagata, 992-8510, Japan
SOURCE: Tetrahedron Letters (2003), 44(45), 8269-8272
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:16553

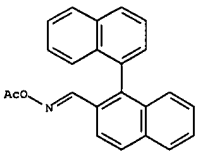
IT **631920-63-3P 631920-66-6P**
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(facile synthesis of chiral formyl binaphthyl via lipase-catalyzed acylation/kinetic resolution and hydrolysis of corresponding binaphthyl oximes)

RN 631920-63-3 CAPLUS
CN [1,1'-Binaphthalene]-2-carboxaldehyde, O-acetyloxime, (1R)- (9CI) (CA INDEX NAME)

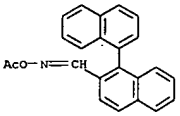


RN 631920-66-6 CAPLUS
CN [1,1'-Binaphthalene]-2-carboxaldehyde, O-acetyloxime, (1S)- (9CI) (CA INDEX NAME)

L19 ANSWER 2 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



IT **630407-82-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(facile synthesis of chiral formyl binaphthyl via lipase-catalyzed acylation/kinetic resolution and hydrolysis of corresponding binaphthyl
oximes)
RN 630407-82-8 CAPLUS
CN [1,1'-Binaphthalene]-2-carboxaldehyde, O-acetyloxime (9CI) (CA INDEX NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

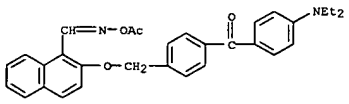
L19 ANSWER 3 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
AB Aromatic compds. having 1 or 2 oxime ester groups such as 1-(6-benzoyl-9-ethyl-9H-carbazolyl)octan-1-one oxime O-acetate (I) are useful as initiators for photopolymn. of unsatd. compds., especially in photoimaging. I was manufactured by stirring CH2Cl2 containing N-ethylcarbazole
7.83, BzCl 5.91, and AlCl3 5.88 g 4 h, adding 6.89 g octanoyl chloride and
5.92 g AlCl3, adding 2.14 g resulting intermediate in EtOH to water containing
0.39 g hydroxylammonium chloride and 0.54 g NaOAc, refluxing 7 h, adding 0.53 g AcCl and then 1 mL Et3N to tert-Bu Me ether containing the 2nd intermediate, and stirring 2.5 h.

ACCESSION NUMBER: 2002:964398 CAPLUS
DOCUMENT NUMBER: 138:47420
TITLE: Aromatic oxime ester photoinitiators
INVENTOR(S): Kunimoto, Kazuhiko; Tanabe, Junichi; Kura, Hisatoshi; Oka, Hidetaka; Ohwa, Masaki
PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.
SOURCE: PCT Int. Appl., 97 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002100903	A1	20021219	WO 2002-EP6107	20020604
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1395615	A1	20040310	EP 2002-778878	20020604
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004534797	T2	20041118	JP 2003-503669	20020604
US 2004170924	A1	20040902	US 2003-480146	20031208
PRIORITY APPLN. INFO.:			EP 2001-810559 A	20010611
			WO 2002-EP6107 W	20020604

OTHER SOURCE(S): MARPAT 138:47420
IT **478556-44-4P**
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(aromatic oxime ester initiators for use in photoimaging compns.)
RN 478556-44-4 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-[[4-[4-(diethylamino)benzoyl]phenyl]methoxy]-, 1-(O-acetyloxime) (9CI) (CA INDEX NAME)

L19 ANSWER 3 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L19 ANSWER 4 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
AB The title compns. are easily applied to a substrate, but yet they possess adequate cohesive strength after application. A method for transitioning a crosslinked polymer composition from a 1st chemical state to a 2nd at least
partially crosslinked chemical state. Thus, acrylic acid-4-acryloxybenzophenone-2-ethylhexyl acrylate-methacrylic acid-2-(5-[2-(hydroxyiminomethyl)phenoxy]pentyloxy)benzaldehyde oxime copolymer crosslinked beads (gel content 66%) were mixed with SiO2, activated at 175°, hot melt pressed between two release liners, and laminated to a functional film, showing a 180° peel adhesion 53.4 N/mm.

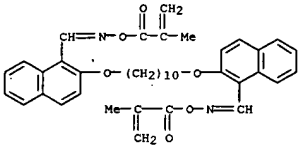
ACCESSION NUMBER: 2002:51555 CAPLUS
DOCUMENT NUMBER: 136:103215
TITLE: Polymer compositions with energetically degradable crosslinker
INVENTOR(S): Everaerts, Albert I.; Leir, Charles M.; Mader, Roger A.; Stark, Peter A.
PATENT ASSIGNEE(S): 3M Innovative Properties Company, USA
SOURCE: PCT Int. Appl., 72 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004548	A1	20020117	WO 2000-US31643	20001109
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:			US 2000-611589 A	20000707

IT **389600-81-1P**
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
((photo)curable polymer compns. with energetically degradable crosslinker for adhesive coatings)
RN 389600-81-1 CAPLUS
CN 2-Propenoic acid, polymer with 2,2'-[1,10-decanediylbis(oxy)]bis[1-naphthalenecarboxaldehyde] bis[O-(2-methyl-1-oxo-2-propenyl)oxime] and isooctyl 2-propenoate (9CI) (CA INDEX NAME)

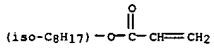
CM 1

CRN 389600-60-6
CMF C40 H44 N2 O6



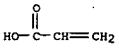
CM 2

CRN 29590-42-9
CMF C11 H20 O2
CCI IDS

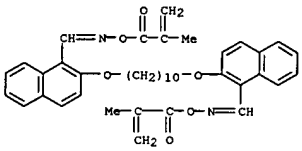


CM 3

CRN 79-10-7
CMF C3 H4 O2



IT **389600-60-6P**
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
(Reactant or reagent)
(crosslinker; (photo)curable polymer compns. with energetically degradable crosslinker for adhesive coatings)
RN 389600-60-6 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2,2'-[1,10-decanediylbis(oxy)]bis-, bis[O-(2-methyl-1-oxo-2-propenyl)oxime] (9CI) (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L19 ANSWER 5 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

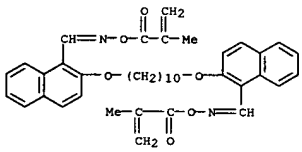
AB A degradable crosslinker comprises: at least one energetically labile moiety and at least two free radically polymerizable groups, wherein the degradable crosslinker is capable of fragmentation into at least two fragments upon activation by an external energy source, wherein the fragments are essentially free of free radicals and ethylenic unsatn. 2-(5-[2-(Hydroxyiminomethyl)phenoxy]pentyloxy) benzaldehyde oxime dimethacrylate ester was prepared as a degradable crosslinker.

ACCESSION NUMBER: 2002:51421 CAPLUS
DOCUMENT NUMBER: 136:103214
TITLE: Degradable crosslinkers, compositions therefrom, and methods of their preparation and use
INVENTOR(S): Everaerts, Albert I.; Leir, Charles M.; Mader, Roger A.; Stark, Peter A.
PATENT ASSIGNEE(S): 3M Innovative Properties Company, USA
SOURCE: PCT Int. Appl., 67 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004408	A1	20020117	WO 2000-US31642	20001109
W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6652970	B1	20031125	US 2000-612016	20000707
EP 1301470	A1	20030416	EP 2000-983720	20001109
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004502837	T2	20040129	JP 2002-509076	20001109

PRIORITY APPLN. INFO.: US 2000-612016 A 20000707
WO 2000-US31642 W 20001109

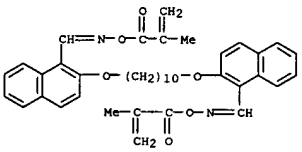
IT **389600-60-6P**
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
(Reactant or reagent)
(crosslinker; degradable crosslinkers, compns. therefrom, and methods of their preparation and use)
RN 389600-60-6 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2,2'-[1,10-decanediylbis(oxy)]bis-, bis[O-(2-methyl-1-oxo-2-propenyl)oxime] (9CI) (CA INDEX NAME)



IT **389600-81-1P**
RL: IMF (Industrial manufacture); PRP (Properties); PREP (Preparation)
(degradable crosslinkers, compns. therefrom, and methods of their preparation and use)
RN 389600-81-1 CAPLUS
CN 2-Propenoic acid, polymer with 2,2'-[1,10-decanediylbis(oxy)]bis[1-naphthalenecarboxaldehyde] bis[O-(2-methyl-1-oxo-2-propenyl)oxime] and isooctyl 2-propenoate (9CI) (CA INDEX NAME)

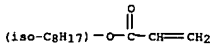
CM 1

CRN 389600-60-6
CMF C40 H44 N2 O6



CM 2

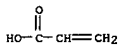
CRN 29590-42-9
CMF C11 H20 O2
CCI IDS



CM 3

CRN 79-10-7
CMF C3 H4 O2

L19 ANSWER 5 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



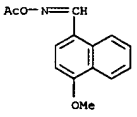
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L19 ANSWER 6 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
(oxime in light-sensitive color filter compn.)

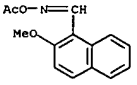
RN 362523-11-3 CAPLUS

CN 1-Naphthalenecarboxaldehyde, 4-methoxy-, O-acetyloxime (9CI) (CA INDEX NAME)



RN 362523-14-6 CAPLUS

CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-acetyloxime (9CI) (CA INDEX NAME)



L19 ANSWER 6 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

AB The title composition contains alkali soluble composition materials, oxime ester as a polymerization initiator, and photopolymg. materials, wherein the oxime ester has structure Ar1-C=NOR1(H) or M1-[-C=NOR1(H)]x (R1 = cycloalkanoyl, benzoyl, alkenoyl; Ar1 = aryl, aroyl; M1 = 2, 3). The composition, which contain the oxime ester, provides the photoresist of the improved resolution and shows the good storageability.

ACCESSION NUMBER: 2001:752027 CAPLUS
DOCUMENT NUMBER: 135:264637
TITLE: Light-sensitive photoresist composition containing oxime esters as polymerization initiator in fabrication of optical filters in optical imaging devices
INVENTOR(S): Oka, Hidetaka; Kunimoto, Kazuhiko; Kura, Hisatoshi; Ohwa, Masaki; Tanabe, Junichi
PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.
SOURCE: Fr. Demande, 110 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2802655	A1	20010622	FR 2000-16309	20001214
FR 2802655	B1	20030815		
SG 97168	A1	20030718	SG 2000-6382	20001103
NL 1016814	A1	20010618	NL 2000-1016814	20001206
NL 1016814	C2	20020129		
GB 2357293	A1	20010620	GB 2000-29801	20001207
GB 2357293	B2	20020807		
SE 2000004565	A	20010725	SE 2000-4565	20001211
SE 522645	C2	20040224		
JP 2001235858	A2	20010831	JP 2000-376036	20001211
US 2002020832	A1	20020221	US 2000-734635	20001212
IT 1319687	B1	20031023	IT 2000-MI2675	20001212
CA 2328342	AA	20010615	CA 2000-2328342	20001213
FI 2000002731	A	20010616	FI 2000-2731	20001213
DE 10061948	A1	20010621	DE 2000-10061948	20001213
BR 2000005866	A	20020521	BR 2000-5866	20001213
CN 1305124	A	20010725	CN 2000-135063	20001214
BE 1013705	A3	20020604	BE 2000-786	20001214
AT 200002080	A5	20020615	AT 2000-2080	20001214
AT 410146	B	20030225		
ES 2189609	A1	20030701	ES 2000-2990	20001214
ES 2189609	B1	20040401		
AU 773749	B2	20040603	AU 2000-72268	20001214

PRIORITY APPLN. INFO.: EP 1999-811161 A 19991215
EP 2000-810630 A 20000717

IT **362523-11-3P 362523-14-6P**
RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

L19 ANSWER 7 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

AB The invention relates to a photopolymn. initiator of oxime ester for a photoresist composition, wherein the oxime is derivative of Ar1-C=N-OR1(H) (R1 = cycloalkanoyl, benzoyl, alkenoyl; Ar1 = aryl, aroyl). The photopolymn. initiator provides the alkali-developable light-sensitive photoresist composition, which shows the improved storageability, of the high resolution and the good storageability.

ACCESSION NUMBER: 2001:752026 CAPLUS
DOCUMENT NUMBER: 135:280493
TITLE: Photopolymerization initiator of oxime ester for light-sensitive photoresist composition
INVENTOR(S): Kunimoto, Kazuhiko; Oka, Hidetaka; Ohwa, Masaki; Tanabe, Junichi; Kura, Hisatoshi; Birbaum, Jean Luc
PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.
SOURCE: Fr. Demande, 171 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

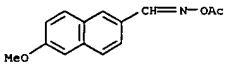
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2802528	A1	20010622	FR 2000-16306	20001214
TW 499411	B	20020821	TW 2000-89123924	20001110
NL 1016815	A1	20010618	NL 2000-1016815	20001206
NL 1016815	C2	20020514		
GB 2358017	A1	20010711	GB 2000-29793	20001207
GB 2358017	B2	20020313		
SE 2000004564	A	20020612	SE 2000-4564	20001211
SE 522774	C2	20040302		
US 2001012596	A1	20010809	US 2000-734625	20001212
JP 2001233842	A2	20010828	JP 2000-377671	20001212
IT 1319688	B1	20031023	IT 2000-MI2676	20001212
CA 2328376	AA	20010615	CA 2000-2328376	20001213
FI 2000002730	A	20010616	FI 2000-2730	20001213
DE 10061947	A1	20010621	DE 2000-10061947	20001213
ES 2177438	A1	20021201	ES 2000-2977	20001213
ES 2177438	B1	20041016		
DK 200001878	A5	20010616	DK 2000-1878	20001214
BE 1013872	A5	20021105	BE 2000-789	20001214
CN 1299812	A	20010620	CN 2000-135980	20001215
BR 2000006379	A	20010724	BR 2000-6379	20001215

PRIORITY APPLN. INFO.: EP 1999-811160 A 19991215
EP 2000-810629 A 20000717

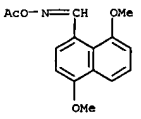
IT **362624-70-2P 362624-71-3P 362624-72-4P**
362624-73-5P 362624-91-7P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(light-sensitive color filter composition containing oxime esters used in optical imaging devices)

RN 362624-70-2 CAPLUS

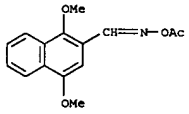
CN 2-Naphthalenecarboxaldehyde, 6-methoxy-, O-acetyloxime (9CI) (CA INDEX NAME)



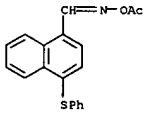
RN 362624-71-3 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 4,8-dimethoxy-, O-acetyloxime (9CI) (CA INDEX NAME)



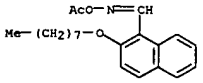
RN 362624-72-4 CAPLUS
CN 2-Naphthalenecarboxaldehyde, 1,4-dimethoxy-, O-acetyloxime (9CI) (CA INDEX NAME)



RN 362624-73-5 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 4-(phenylthio)-, O-acetyloxime (9CI) (CA INDEX NAME)



RN 362624-91-7 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-(octyloxy)-, O-acetyloxime (9CI) (CA INDEX NAME)



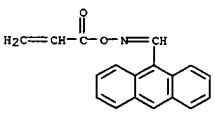
L19 ANSWER 8 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

AB Antireflective films suitable for submicron lithog. and the production of semiconductor elements contain acrylic polymers with anthracenecarboxaldehyde oxime chromophore units. The polymers are prepared by radical polymerization with other acrylic monomers. Back reflections of light and the problem of the critical dimension change, which are due to scattered and/or reflected light, are reduced clearly or avoided by the antireflective films. The effect of a standing wave and of reflection grooves are reduced or eliminated. In an example, 9-anthracenecarboxaldehyde oxime was condensed with acryloyl chloride to give a monomer, which was copolymd. with 2-hydroxyethyl acrylate to give a polymer which could be combined with acetals of polyacrolein or polymethacrolein to give antireflective film materials.

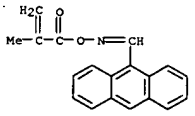
ACCESSION NUMBER: 2001:467935 CAPLUS
DOCUMENT NUMBER: 135:77875
TITLE: Antireflective films containing anthracene-based acrylic polymers, their production and their use
INVENTOR(S): Jung, Min-Ho; Hong, Sung-Eun; Jung, Jae-Chang; Lee, Geun-Su; Baik, Ki-Ho
PATENT ASSIGNEE(S): Hyundai Electronics Industries Co., Ltd., S. Korea
SOURCE: Ger. Offen., 18 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10063263	A1	20010628	DE 2000-10063263	20001219
KR 2001057925	A	20010705	KR 1999-61344	19991223
NL 1016942	A1	20010626	NL 2000-1016942	20001221
NL 1016942	C2	20020501		
JP 2001192422	A2	20010717	JP 2000-388729	20001221
GB 2357511	A1	20010627	GB 2000-31419	20001222
GB 2357511	B2	20030402		
FR 2802935	A1	20010629	FR 2000-16962	20001222
FR 2802935	B1	20030328		
US 2001034427	A1	20011025	US 2000-747364	20001222
US 6548613	B2	20030415		
IT 1320867	B1	20031210	IT 2000-TO1220	20001222
CN 1308089	A	20010815	CN 2000-136237	20001225
FR 2808027	A1	20011026	FR 2001-6011	20010504
PRIORITY APPLN. INFO.:			KR 1999-61344 A	19991223

OTHER SOURCE(S): MARPAT 135:77875
IT **330443-03-3P**, 9-Anthracenecarboxaldehyde oxime acrylate
330443-05-5P, 9-Anthracenecarboxaldehyde oxime methacrylate
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(monomer; production of anthracenecarboxaldehyde oxime-based acrylic polymers for antireflective films)
RN 330443-03-3 CAPLUS
CN 9-Anthracenecarboxaldehyde, O-(1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)



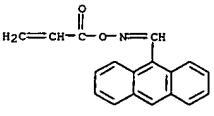
RN 330443-05-5 CAPLUS
CN 9-Anthracenecarboxaldehyde, O-(2-methyl-1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)



IT **346685-19-6P 346685-20-9P 346685-21-0P**
346685-22-1P 346685-23-2P 346685-24-3P
346685-25-4P 346685-26-5P 346685-27-6P
346685-28-7P 346685-29-8P 346685-30-1P
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(production of anthracenecarboxaldehyde oxime-based acrylic polymers for antireflective films)
RN 346685-19-6 CAPLUS
CN 2-Propenoic acid, 2-hydroxyethyl ester, polymer with 9-anthracenecarboxaldehyde O-(1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)

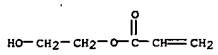
CM 1

CRN 330443-03-3
CMF C18 H13 N O2



CM 2

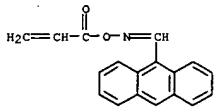
L19 ANSWER 8 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CRN 818-61-1
CMF C5 H8 O3



RN 346685-20-9 CAPLUS
CN 2-Propenoic acid, 3-hydroxypropyl ester, polymer with 9-anthracenecarboxaldehyde O-(1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)

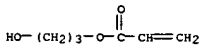
CM 1

CRN 330443-03-3
CMF C18 H13 N O2



CM 2

CRN 2761-08-2
CMF C6 H10 O3



RN 346685-21-0 CAPLUS
CN 2-Propenoic acid, 4-hydroxybutyl ester, polymer with 9-anthracenecarboxaldehyde O-(1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)

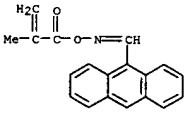
CM 1

CRN 330443-03-3
CMF C18 H13 N O2

L19 ANSWER 8 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
INDEX NAME)

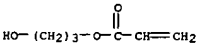
CM 1

CRN 330443-05-5
CMF C19 H15 N O2



CM 2

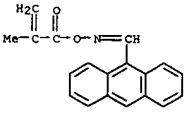
CRN 2761-08-2
CMF C6 H10 O3



RN 346685-24-3 CAPLUS
CN 2-Propenoic acid, 4-hydroxybutyl ester, polymer with 9-anthracenecarboxaldehyde O-(2-methyl-1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)

CM 1

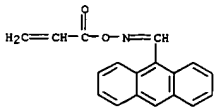
CRN 330443-05-5
CMF C19 H15 N O2



CM 2

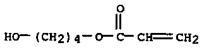
CRN 2478-10-6
CMF C7 H12 O3

L19 ANSWER 8 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



CM 2

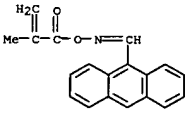
CRN 2478-10-6
CMF C7 H12 O3



RN 346685-22-1 CAPLUS
CN 2-Propenoic acid, 2-hydroxyethyl ester, polymer with 9-anthracenecarboxaldehyde O-(2-methyl-1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)

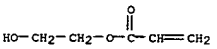
CM 1

CRN 330443-05-5
CMF C19 H15 N O2



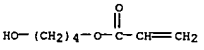
CM 2

CRN 818-61-1
CMF C5 H8 O3



RN 346685-23-2 CAPLUS
CN 2-Propenoic acid, 3-hydroxypropyl ester, polymer with 9-anthracenecarboxaldehyde O-(2-methyl-1-oxo-2-propenyl)oxime (9CI) (CA

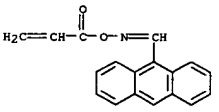
L19 ANSWER 8 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 346685-25-4 CAPLUS
CN 2-Propenoic acid, 2-methyl-, methyl ester, polymer with 9-anthracenecarboxaldehyde O-(1-oxo-2-propenyl)oxime and 2-hydroxyethyl 2-propenoate (9CI) (CA INDEX NAME)

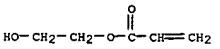
CM 1

CRN 330443-03-3
CMF C18 H13 N O2



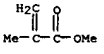
CM 2

CRN 818-61-1
CMF C5 H8 O3



CM 3

CRN 80-62-6
CMF C5 H8 O2

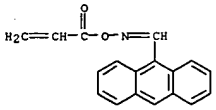


RN 346685-26-5 CAPLUS
CN 2-Propenoic acid, 2-methyl-, methyl ester, polymer with 9-anthracenecarboxaldehyde O-(1-oxo-2-propenyl)oxime and 3-hydroxypropyl 2-propenoate (9CI) (CA INDEX NAME)

CM 1

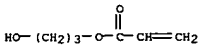
CRN 330443-03-3

L19 ANSWER 8 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CMF C18 H13 N O2



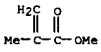
CM 2

CRN 2761-08-2
CMF C6 H10 O3



CM 3

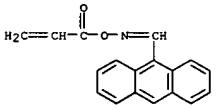
CRN 80-62-6
CMF C5 H8 O2



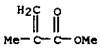
RN 346685-27-6 CAPLUS
CN 2-Propenoic acid, 2-methyl-, methyl ester, polymer with 9-anthracenecarboxaldehyde O-(1-oxo-2-propenyl)oxime and 4-hydroxybutyl 2-propenoate (9CI) (CA INDEX NAME)

CM 1

CRN 330443-03-3
CMF C18 H13 N O2



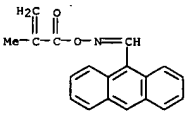
L19 ANSWER 8 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CRN 80-62-6
CMF C5 H8 O2



RN 346685-29-8 CAPLUS
CN 2-Propenoic acid, 2-methyl-, methyl ester, polymer with 9-anthracenecarboxaldehyde O-(2-methyl-1-oxo-2-propenyl)oxime and 3-hydroxypropyl 2-propenoate (9CI) (CA INDEX NAME)

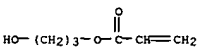
CM 1

CRN 330443-05-5
CMF C19 H15 N O2



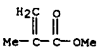
CM 2

CRN 2761-08-2
CMF C6 H10 O3



CM 3

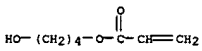
CRN 80-62-6
CMF C5 H8 O2



RN 346685-30-1 CAPLUS
CN 2-Propenoic acid, 2-methyl-, methyl ester, polymer with 9-anthracenecarboxaldehyde O-(2-methyl-1-oxo-2-propenyl)oxime and 4-hydroxybutyl 2-propenoate (9CI) (CA INDEX NAME)

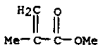
L19 ANSWER 8 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CM 2

CRN 2478-10-6
CMF C7 H12 O3



CM 3

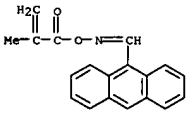
CRN 80-62-6
CMF C5 H8 O2



RN 346685-28-7 CAPLUS
CN 2-Propenoic acid, 2-methyl-, methyl ester, polymer with 9-anthracenecarboxaldehyde O-(2-methyl-1-oxo-2-propenyl)oxime and 2-hydroxyethyl 2-propenoate (9CI) (CA INDEX NAME)

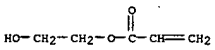
CM 1

CRN 330443-05-5
CMF C19 H15 N O2



CM 2

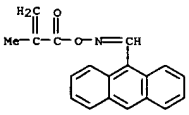
CRN 818-61-1
CMF C5 H8 O3



CM 3

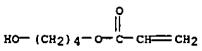
L19 ANSWER 8 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CM 1

CRN 330443-05-5
CMF C19 H15 N O2



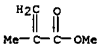
CM 2

CRN 2478-10-6
CMF C7 H12 O3



CM 3

CRN 80-62-6
CMF C5 H8 O2



L19 ANSWER 9 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

AB Acrylate and methacrylate esters of 9-anthracenecarboxaldehyde oxime are prepared and radically copolymd. in solution with other acrylic monomers to provide products suitable for use as antireflective coatings for integrated circuit semiconductor materials and laser submicron lithog. In an example, 9-anthracenecarboxaldehyde oxime acrylate was prepared from the acid chloride and copolymd. with 2-hydroxyethyl acrylate and glycidyl methacrylate.

ACCESSION NUMBER: 2001:238137 CAPLUS
DOCUMENT NUMBER: 134:237981
TITLE: 9-Anthraldehyde oxime (meth)acrylates, their production, and polymers for antireflecting coatings therefrom
INVENTOR(S): Jung, Min Ho; Hong, Sung Eun; Baik, Ki Ho
PATENT ASSIGNEE(S): Hyundai Electronics Industries Co. Ltd., S. Korea
SOURCE: Fr. Demande, 36 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

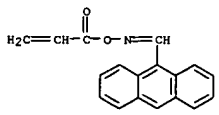
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2795411	A1	20001229	FR 2000-7853	20000620
FR 2795411	B1	20040130		
KR 2001003188	A	20010115	KR 1999-23382	19990622
TW 553923	B	20030921	TW 2000-89110845	20000603
DE 10028345	A1	20010125	DE 2000-10028345	20000608
GB 2351288	A1	20001227	GB 2000-14257	20000613
GB 2351288	B2	20040211		
NL 1015471	A1	20001228	NL 2000-1015471	20000619
NL 1015471	C2	20010409		
JP 2001049231	A2	20010220	JP 2000-182834	20000619
CN 1278529	A	20010103	CN 2000-107842	20000622
US 6388039	B1	20020514	US 2000-602655	20000622
US 2002136834	A1	20020926	US 2002-95417	20020311
US 6538090	B2	20030325		
US 2002137826	A1	20020926	US 2002-95852	20020311
US 6489423	B2	20021203		

PRIORITY APPLN. INFO.: KR 1999-23382 A 19990622
US 2000-602655 A3 20000622

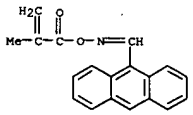
OTHER SOURCE(S): MARPAT 134:237981

IT **330443-03-3P**, 9-Anthracenecarboxaldehyde oxime acrylate
330443-05-5P, 9-Anthracenecarboxaldehyde oxime methacrylate
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(monomer; production and polymerization of anthracenecarboxaldehyde oxime (meth)acrylates for antireflective coatings)

RN 330443-03-3 CAPLUS
CN 9-Anthracenecarboxaldehyde, O-(1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)



RN 330443-05-5 CAPLUS
CN 9-Anthracenecarboxaldehyde, O-(2-methyl-1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)



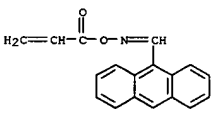
IT **330443-07-7P**, 9-Anthracenecarboxaldehyde oxime acrylate-glycidyl methacrylate-2-hydroxyethyl acrylate copolymer **330443-09-9P**, 9-Anthracenecarboxaldehyde oxime acrylate-glycidyl methacrylate-3-hydroxypropyl acrylate copolymer **330443-11-3P**, 9-Anthracenecarboxaldehyde oxime acrylate-glycidyl acrylate-2-hydroxyethyl acrylate copolymer **330443-13-5P**, 9-Anthracenecarboxaldehyde oxime acrylate-glycidyl acrylate-3-hydroxypropyl acrylate copolymer **330443-15-7P**, 9-Anthracenecarboxaldehyde oxime acrylate-glycidyl acrylate-4-hydroxybutyl acrylate copolymer **330443-17-9P**, 9-Anthracenecarboxaldehyde oxime methacrylate-glycidyl methacrylate-2-hydroxyethyl acrylate copolymer **330443-18-0P**, 9-Anthracenecarboxaldehyde oxime methacrylate-glycidyl methacrylate-3-hydroxypropyl acrylate copolymer **330443-19-1P**, 9-Anthracenecarboxaldehyde oxime methacrylate-glycidyl methacrylate-4-hydroxybutyl acrylate copolymer **330443-21-5P**, 9-Anthracenecarboxaldehyde oxime methacrylate-glycidyl acrylate-2-hydroxyethyl acrylate copolymer **330443-23-7P**, 9-Anthracenecarboxaldehyde oxime methacrylate-glycidyl acrylate-3-hydroxypropyl acrylate copolymer **330443-25-9P**, 9-Anthracenecarboxaldehyde oxime methacrylate-glycidyl acrylate-4-hydroxybutyl acrylate copolymer **330443-26-0P**, 9-Anthracenecarboxaldehyde oxime acrylate-glycidyl methacrylate-2-hydroxyethyl acrylate-methyl methacrylate copolymer **330443-27-1P**, 9-Anthracenecarboxaldehyde oxime acrylate-glycidyl methacrylate-3-hydroxypropyl acrylate-methyl methacrylate copolymer **330443-28-2P**, 9-Anthracenecarboxaldehyde oxime acrylate-glycidyl acrylate-2-hydroxyethyl acrylate-methyl methacrylate copolymer **330443-29-3P**, 9-Anthracenecarboxaldehyde oxime acrylate-glycidyl acrylate-3-hydroxypropyl acrylate-methyl methacrylate copolymer **330443-30-6P**, 9-Anthracenecarboxaldehyde oxime acrylate-glycidyl acrylate-4-hydroxybutyl acrylate-methyl methacrylate copolymer **330443-31-7P**, 9-Anthracenecarboxaldehyde oxime methacrylate-glycidyl

methacrylate-2-hydroxyethyl acrylate-methyl methacrylate copolymer **330443-32-8P**, 9-Anthracenecarboxaldehyde oxime methacrylate-glycidyl methacrylate-3-hydroxypropyl acrylate-methyl methacrylate copolymer **330443-33-9P**, 9-Anthracenecarboxaldehyde oxime methacrylate-glycidyl methacrylate-4-hydroxybutyl acrylate-methyl methacrylate copolymer **330443-34-0P**, 9-Anthracenecarboxaldehyde oxime methacrylate-glycidyl acrylate-2-hydroxyethyl acrylate-methyl methacrylate copolymer **330443-35-1P**, 9-Anthracenecarboxaldehyde oxime methacrylate-glycidyl acrylate-3-hydroxypropyl acrylate-methyl methacrylate copolymer **330443-36-2P**, 9-Anthracenecarboxaldehyde oxime methacrylate-glycidyl acrylate-4-hydroxybutyl acrylate-methyl methacrylate copolymer
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(prodn. of anthracenecarboxaldehyde oxime (meth)acrylate copolymers for antireflective coatings)

RN 330443-07-7 CAPLUS
CN 2-Propenoic acid, 2-methyl-, oxiranylmethyl ester, polymer with 9-anthracenecarboxaldehyde O-(1-oxo-2-propenyl)oxime and 2-hydroxyethyl 2-propenoate (9CI) (CA INDEX NAME)

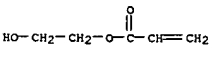
CM 1

CRN 330443-03-3
CMF C18 H13 N O2



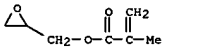
CM 2

CRN 818-61-1
CMF C5 H8 O3



CM 3

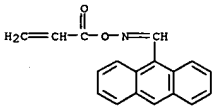
CRN 106-91-2
CMF C7 H10 O3



RN 330443-09-9 CAPLUS
CN 2-Propenoic acid, 2-methyl-, oxiranylmethyl ester, polymer with 9-anthracenecarboxaldehyde O-(1-oxo-2-propenyl)oxime and 3-hydroxypropyl 2-propenoate (9CI) (CA INDEX NAME)

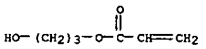
CM 1

CRN 330443-03-3
CMF C18 H13 N O2



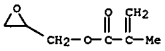
CM 2

CRN 2761-08-2
CMF C6 H10 O3



CM 3

CRN 106-91-2
CMF C7 H10 O3

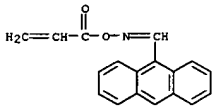


RN 330443-11-3 CAPLUS
CN 2-Propenoic acid, 2-hydroxyethyl ester, polymer with 9-anthracenecarboxaldehyde O-(1-oxo-2-propenyl)oxime and oxiranylmethyl 2-propenoate (9CI) (CA INDEX NAME)

CM 1

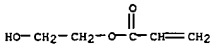
CRN 330443-03-3

L19 ANSWER 9 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CMF C18 H13 N O2



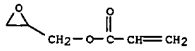
CM 2

CRN 818-61-1
CMF C5 H8 O3



CM 3

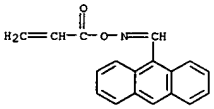
CRN 106-90-1
CMF C6 H8 O3



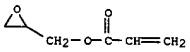
RN 330443-13-5 CAPLUS
CN 2-Propenoic acid, 3-hydroxypropyl ester, polymer with 9-anthracenecarboxaldehyde O-(1-oxo-2-propenyl)oxime and oxiranylmethyl 2-propenoate (9CI) (CA INDEX NAME)

CM 1

CRN 330443-03-3
CMF C18 H13 N O2



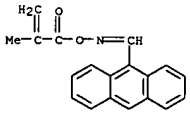
L19 ANSWER 9 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CRN 106-90-1
CMF C6 H8 O3



RN 330443-17-9 CAPLUS
CN 2-Propenoic acid, 2-methyl-, oxiranylmethyl ester, polymer with 9-anthracenecarboxaldehyde O-(2-methyl-1-oxo-2-propenyl)oxime and 2-hydroxyethyl 2-propenoate (9CI) (CA INDEX NAME)

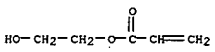
CM 1

CRN 330443-05-5
CMF C19 H15 N O2



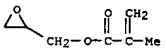
CM 2

CRN 818-61-1
CMF C5 H8 O3



CM 3

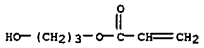
CRN 106-91-2
CMF C7 H10 O3



RN 330443-18-0 CAPLUS
CN 2-Propenoic acid, 2-methyl-, oxiranylmethyl ester, polymer with 9-anthracenecarboxaldehyde O-(2-methyl-1-oxo-2-propenyl)oxime and 3-hydroxypropyl 2-propenoate (9CI) (CA INDEX NAME)

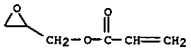
L19 ANSWER 9 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CM 2

CRN 2761-08-2
CMF C6 H10 O3



CM 3

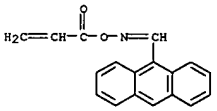
CRN 106-90-1
CMF C6 H8 O3



RN 330443-15-7 CAPLUS
CN 2-Propenoic acid, 4-hydroxybutyl ester, polymer with 9-anthracenecarboxaldehyde O-(1-oxo-2-propenyl)oxime and oxiranylmethyl 2-propenoate (9CI) (CA INDEX NAME)

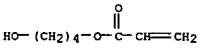
CM 1

CRN 330443-03-3
CMF C18 H13 N O2



CM 2

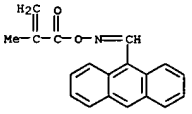
CRN 2478-10-6
CMF C7 H12 O3



CM 3

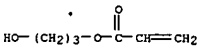
L19 ANSWER 9 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CM 1

CRN 330443-05-5
CMF C19 H15 N O2



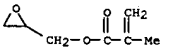
CM 2

CRN 2761-08-2
CMF C6 H10 O3



CM 3

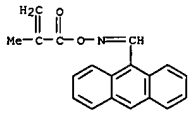
CRN 106-91-2
CMF C7 H10 O3



RN 330443-19-1 CAPLUS
CN 2-Propenoic acid, 2-methyl-, oxiranylmethyl ester, polymer with 9-anthracenecarboxaldehyde O-(2-methyl-1-oxo-2-propenyl)oxime and 4-hydroxybutyl 2-propenoate (9CI) (CA INDEX NAME)

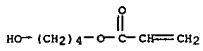
CM 1

CRN 330443-05-5
CMF C19 H15 N O2



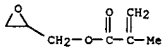
CM 2

CRN 2478-10-6
CMF C7 H12 O3



CM 3

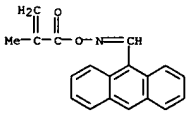
CRN 106-91-2
CMF C7 H10 O3



RN 330443-21-5 CAPLUS
CN 2-Propenoic acid, 2-hydroxyethyl ester, polymer with 9-anthracenecarboxaldehyde O-(2-methyl-1-oxo-2-propenyl)oxime and oxiranylmethyl 2-propenoate (9CI) (CA INDEX NAME)

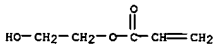
CM 1

CRN 330443-05-5
CMF C19 H15 N O2



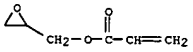
CM 2

CRN 818-61-1
CMF C5 H8 O3



CM 3

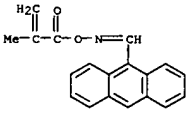
CRN 106-90-1
CMF C6 H8 O3



RN 330443-23-7 CAPLUS
CN 2-Propenoic acid, 3-hydroxypropyl ester, polymer with 9-anthracenecarboxaldehyde O-(2-methyl-1-oxo-2-propenyl)oxime and oxiranylmethyl 2-propenoate (9CI) (CA INDEX NAME)

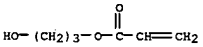
CM 1

CRN 330443-05-5
CMF C19 H15 N O2



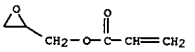
CM 2

CRN 2761-08-2
CMF C6 H10 O3



CM 3

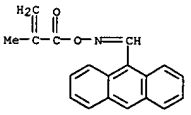
CRN 106-90-1
CMF C6 H8 O3



RN 330443-25-9 CAPLUS
CN 2-Propenoic acid, 4-hydroxybutyl ester, polymer with 9-anthracenecarboxaldehyde O-(2-methyl-1-oxo-2-propenyl)oxime and oxiranylmethyl 2-propenoate (9CI) (CA INDEX NAME)

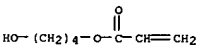
CM 1

CRN 330443-05-5
CMF C19 H15 N O2



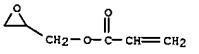
CM 2

CRN 2478-10-6
CMF C7 H12 O3



CM 3

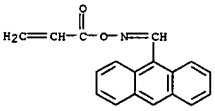
CRN 106-90-1
CMF C6 H8 O3



RN 330443-26-0 CAPLUS
CN 2-Propenoic acid, 2-methyl-, methyl ester, polymer with 9-anthracenecarboxaldehyde O-(1-oxo-2-propenyl)oxime, 2-hydroxyethyl 2-propenoate and oxiranylmethyl 2-methyl-2-propenoate (9CI) (CA INDEX NAME)

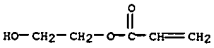
CM 1

CRN 330443-03-3
CMF C18 H13 N O2



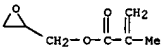
CM 2

CRN 818-61-1
CMF C5 H8 O3



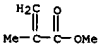
CM 3

CRN 106-91-2
CMF C7 H10 O3



CM 4

CRN 80-62-6
CMF C5 H8 O2

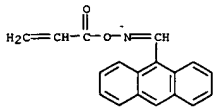


RN 330443-27-1 CAPLUS
CN 2-Propenoic acid, 2-methyl-, methyl ester, polymer with 9-anthracenecarboxaldehyde O-(1-oxo-2-propenyl)oxime, 3-hydroxypropyl 2-propenoate and oxiranylmethyl 2-methyl-2-propenoate (9CI) (CA INDEX NAME)

CM 1

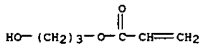
L19 ANSWER 9 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

CRN 330443-03-3
CMF C18 H13 N O2



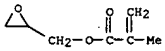
CM 2

CRN 2761-08-2
CMF C6 H10 O3



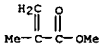
CM 3

CRN 106-91-2
CMF C7 H10 O3



CM 4

CRN 80-62-6
CMF C5 H8 O2

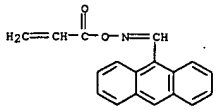


RN 330443-28-2 CAPLUS
CN 2-Propenoic acid, 2-methyl-, methyl ester, polymer with 9-anthracenecarboxaldehyde O-(1-oxo-2-propenyl)oxime, 2-hydroxyethyl 2-propenoate and oxiranylmethyl 2-propenoate (9CI) (CA INDEX NAME)

CM 1

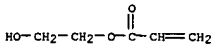
CRN 330443-03-3
CMF C18 H13 N O2

L19 ANSWER 9 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



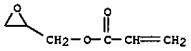
CM 2

CRN 818-61-1
CMF C5 H8 O3



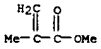
CM 3

CRN 106-90-1
CMF C6 H8 O3



CM 4

CRN 80-62-6
CMF C5 H8 O2

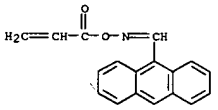


RN 330443-29-3 CAPLUS
CN 2-Propenoic acid, 2-methyl-, methyl ester, polymer with 9-anthracenecarboxaldehyde O-(1-oxo-2-propenyl)oxime, 3-hydroxypropyl 2-propenoate and oxiranylmethyl 2-propenoate (9CI) (CA INDEX NAME)

CM 1

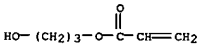
CRN 330443-03-3
CMF C18 H13 N O2

L19 ANSWER 9 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



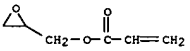
CM 2

CRN 2761-08-2
CMF C6 H10 O3



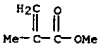
CM 3

CRN 106-90-1
CMF C6 H8 O3



CM 4

CRN 80-62-6
CMF C5 H8 O2

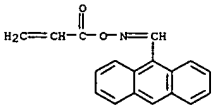


RN 330443-30-6 CAPLUS
CN 2-Propenoic acid, 2-methyl-, methyl ester, polymer with 9-anthracenecarboxaldehyde O-(1-oxo-2-propenyl)oxime, 4-hydroxybutyl 2-propenoate and oxiranylmethyl 2-propenoate (9CI) (CA INDEX NAME)

CM 1

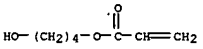
CRN 330443-03-3
CMF C18 H13 N O2

L19 ANSWER 9 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



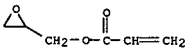
CM 2

CRN 2478-10-6
CMF C7 H12 O3



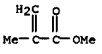
CM 3

CRN 106-90-1
CMF C6 H8 O3



CM 4

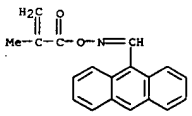
CRN 80-62-6
CMF C5 H8 O2



RN 330443-31-7 CAPLUS
CN 2-Propenoic acid, 2-methyl-, methyl ester, polymer with 9-anthracenecarboxaldehyde O-(2-methyl-1-oxo-2-propenyl)oxime, 2-hydroxyethyl 2-propenoate and oxiranylmethyl 2-methyl-2-propenoate (9CI)
(CA INDEX NAME)

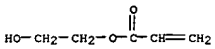
CM 1

CRN 330443-05-5
CMF C19 H15 N O2



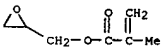
CM 2

CRN 818-61-1
CMF C5 H8 O3



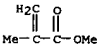
CM 3

CRN 106-91-2
CMF C7 H10 O3



CM 4

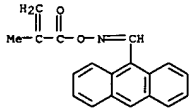
CRN 80-62-6
CMF C5 H8 O2



RN 330443-32-8 CAPLUS
CN 2-Propenoic acid, 2-methyl-, methyl ester, polymer with 9-anthracenecarboxaldehyde O-(2-methyl-1-oxo-2-propenyl)oxime, 3-hydroxypropyl 2-propenoate and oxiranylmethyl 2-methyl-2-propenoate (9CI) (CA INDEX NAME)

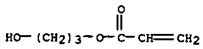
CM 1

CRN 330443-05-5
CMF C19 H15 N O2



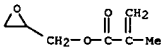
CM 2

CRN 2761-08-2
CMF C6 H10 O3



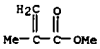
CM 3

CRN 106-91-2
CMF C7 H10 O3



CM 4

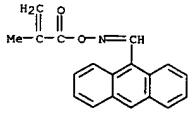
CRN 80-62-6
CMF C5 H8 O2



RN 330443-33-9 CAPLUS
CN 2-Propenoic acid, 2-methyl-, methyl ester, polymer with 9-anthracenecarboxaldehyde O-(2-methyl-1-oxo-2-propenyl)oxime, 4-hydroxybutyl 2-propenoate and oxiranylmethyl 2-methyl-2-propenoate (9CI) (CA INDEX NAME)

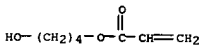
CM 1

CRN 330443-05-5
CMF C19 H15 N O2



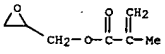
CM 2

CRN 2478-10-6
CMF C7 H12 O3



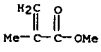
CM 3

CRN 106-91-2
CMF C7 H10 O3



CM 4

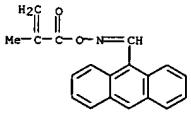
CRN 80-62-6
CMF C5 H8 O2



RN 330443-34-0 CAPLUS
CN 2-Propenoic acid, 2-methyl-, methyl ester, polymer with 9-anthracenecarboxaldehyde O-(2-methyl-1-oxo-2-propenyl)oxime, 2-hydroxyethyl 2-propenoate and oxiranylmethyl 2-propenoate (9CI) (CA INDEX NAME)

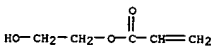
CM 1

CRN 330443-05-5
CMF C19 H15 N O2



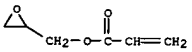
CM 2

CRN 818-61-1
CMF C5 H8 O3



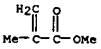
CM 3

CRN 106-90-1
CMF C6 H8 O3



CM 4

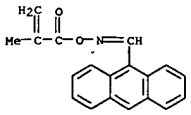
CRN 80-62-6
CMF C5 H8 O2



RN 330443-35-1 CAPLUS
CN 2-Propenoic acid, 2-methyl-, methyl ester, polymer with 9-anthracenecarboxaldehyde O-(2-methyl-1-oxo-2-propenyl)oxime, 3-hydroxypropyl 2-propenoate and oxiranylmethyl 2-propenoate (9CI) (CA INDEX NAME)

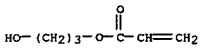
CM 1

CRN 330443-05-5
CMF C19 H15 N O2



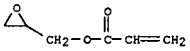
CM 2

CRN 2761-08-2
CMF C6 H10 O3



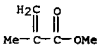
CM 3

CRN 106-90-1
CMF C6 H8 O3



CM 4

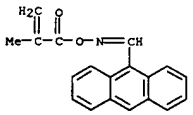
CRN 80-62-6
CMF C5 H8 O2



RN 330443-36-2 CAPLUS
CN 2-Propenoic acid, 2-methyl-, methyl ester, polymer with 9-anthracenecarboxaldehyde O-(2-methyl-1-oxo-2-propenyl)oxime, 4-hydroxybutyl 2-propenoate and oxiranylmethyl 2-propenoate (9CI) (CA INDEX NAME)

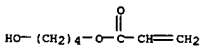
CM 1

CRN 330443-05-5
CMF C19 H15 N O2



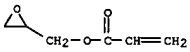
CM 2

CRN 2478-10-6
CMF C7 H12 O3



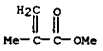
CM 3

CRN 106-90-1
CMF C6 H8 O3



CM 4

CRN 80-62-6
CMF C5 H8 O2

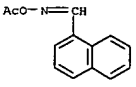


AB Treatment of oxime O-acetates with Co2(CO)8 in the presence of a base, followed by H2O at room temperature efficiently afforded the parent carbonyl compds. in high yields. Direct regeneration of carbonyl functionalities from the corresponding oxime derivs. was realized by successive exposure to acetylation conditions, Co2(CO)8 in the presence of base, and H2O. In addition, N-monosubstituted hydrazones could generate the parent carbonyl compound under the above conditions.

ACCESSION NUMBER: 1999:727404 CAPLUS
DOCUMENT NUMBER: 131:351055
TITLE: Dicobaltoctacarbonyl-mediated deoximation
AUTHOR(S): Mukai, Chisato; Nomura, Izumi; Kataoka, Osamu; Hanaoka, Miyoji
CORPORATE SOURCE: Faculty Pharmaceutical Sciences, Kanazawa Univ., Kanazawa, 920, Japan
SOURCE: Synthesis (1999), (11), 1872-1874
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:351055

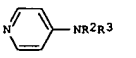
IT **250293-43-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cobaltcarbonyl-mediated deoximation)

RN 250293-43-7 CAPLUS
CN 1-Naphthalenecarboxaldehyde, O-acetyloxime (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

GI



IV

AB R1CH:NOC(O)OR4 [I; R1 = acyl, (substituted) hydrocarbyl, (substituted) heterocyclyl; R4 = alkyl, alkenyl, aralkyl] are prepared by reaction of R1CH:NOH (II; R1 = same as I) with R4OC(O)OC(O)OR4 (III; R4 = same as I) in presence of 0.01-5 mol.% (based on II) aminopyridines IV (R2, R3 = alkyl, aryl; R2R3 may form ring). II (R1 = Ph) was treated with III (R4 = CMe3) and IV (R2 = R3 = Me) in CH2Cl2 at 20° for 8 h to give 97.7% I (R1 = Ph, R4 = CMe3).

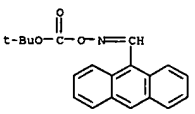
ACCESSION NUMBER: 1996:523557 CAPLUS
DOCUMENT NUMBER: 125:167339
TITLE: Preparation of aldoxime carbonates
INVENTOR(S): Iwasaki, Fumiaki; Mitsuharu, Michiko
PATENT ASSIGNEE(S): Tokuyama Corp, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08151357	A2	19960611	JP 1994-291593	19941125
JP 3295258	B2	20020624		
PRIORITY APPLN. INFO.:			JP 1994-291593	19941125

OTHER SOURCE(S): CASREACT 125:167339; MARPAT 125:167339

IT **180308-34-3P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of aldoxime carbonates from aldoximes and dicarbonates with aminopyridine catalysts)

RN 180308-34-3 CAPLUS
CN 9-Anthracenecarboxaldehyde, O-[(1,1-dimethylethoxy)carbonyl]oxime (9CI) (CA INDEX NAME)



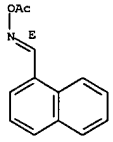
L19 ANSWER 11 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

L19 ANSWER 12 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

AB Aldoximes and some new ether oximes of 1- and 2-naphthaldehyde were prepared by oximation of the corresponding aldehyde followed by O-alkylation in polar media. They were fully characterized by their 1H and 13C NMR spectra (a rapid and systematic approach of their configuration was obtained). The configuration of the C:N double bond was E for the oximes and their ether derivs. Oxime ethers of 2-pyridinecarboxaldehyde oxime and 1,3-benzodioxole-5-carboxaldehyde oxime were also prepared and characterized by NMR and IR spectra. The four oxime ethers studied were also O-acetylated.

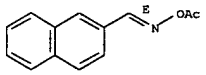
ACCESSION NUMBER: 1994:322894 CAPLUS
DOCUMENT NUMBER: 120:322894
TITLE: Synthesis and C:N double bond stereochemistry of oxime ethers. O-Alkyl oxime ethers of 1- and 2-naphthaldehydes
AUTHOR(S): Dinia, M. N.; Hassikou, A.; Lattes, A.
CORPORATE SOURCE: Lab. Chim. Org., Fac. Sci., Rabat, Morocco
SOURCE: Bulletin des Societes Chimiques Belges (1993), 102(9), 623-4
CODEN: BSCBAG; ISSN: 0037-9646
DOCUMENT TYPE: Journal
LANGUAGE: French
IT **51874-00-1P 51874-01-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 51874-00-1 CAPLUS
CN 1-Naphthalenecarboxaldehyde, O-acetyloxime, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 51874-01-2 CAPLUS
CN 2-Naphthalenecarboxaldehyde, O-acetyloxime, (E)- (9CI) (CA INDEX NAME)

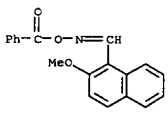
Double bond geometry as shown.



L19 ANSWER 13 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

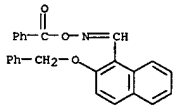
AB Thermal decomposition of syn-RCH:NOCONMe2 [I: R = 2-pyridyl, 4-C6H4NO2, Ph, 4-C6H4NMe2, 2,4- or 2,5-C6H3(OMe)2, 2-methyl- or 2-methoxy-4-dimethylaminophenyl, 2-methoxy-1-naphthyl] and syn-RCH:NOBz [II: R = Ph, 4-C6H4OMe, 2,4-C6H3(OMe)2, 2- or 4-methoxy-1-naphthyl, 1,5-C10H6SO2NEt2, 2-benzyloxy-1-naphthyl] at 80-130° was kinetically studied. The decomposition was 1st-order for both I and II, and electron donating groups and substituents at the ortho position increased the reaction rates. Activation entropy values for I and II were very different and, hence, different decomposition mechanisms were proposed: β-elimination with syn/anti isomerization for I and concerted elimination via a cyclic 6-membered ring transition for II.

ACCESSION NUMBER: 1992:469340 CAPLUS
DOCUMENT NUMBER: 117:69340
TITLE: Reaction control of thermal decomposition of aromatic aldoxime derivatives as heat decomposing precursor compounds
AUTHOR(S): Kawata, Ken; Kitaguchi, Hiroshi; Sato, Kozo; Yabuki, Yoshiharu
CORPORATE SOURCE: Ashigara Res. Lab., Fuji Photo Film Co., Ltd., Kanagawa, 250-01, Japan
SOURCE: Senryo to Yakuhin (1992), 37(2), 33-40
CODEN: SETYAL; ISSN: 0370-9671
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
IT **99806-90-3 100906-56-7 142554-05-0 142554-06-1 142554-07-2**
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(thermal decomposition of, kinetics of, substituent effect and mechanism in relation to)
RN 99806-90-3 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-benzoyloxime (9CI) (CA INDEX NAME)

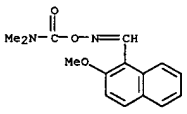


RN 100906-56-7 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-(phenylmethoxy)-, O-benzoyloxime (9CI) (CA INDEX NAME)

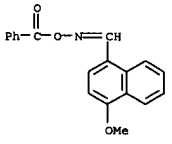
L19 ANSWER 13 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 142554-05-0 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-[(dimethylamino)carbonyl]oxime (9CI) (CA INDEX NAME)

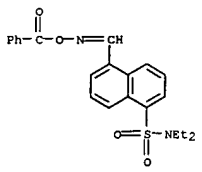


RN 142554-06-1 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 4-methoxy-, O-benzoyloxime (9CI) (CA INDEX NAME)



RN 142554-07-2 CAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(benzoyloxy)imino]methyl]-N,N-diethyl- (9CI)
(CA INDEX NAME)

L19 ANSWER 13 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L19 ANSWER 14 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

AB Eosin-sensitized, laser-induced oxime acrylate sensitizer homo- and copolymn. with polyfunctional acrylates followed by UV crosslinking of the acyloxyimino pendent groups was studied. Photopolymerizability of the various oxime acrylates with and without conventional acrylates was determined using an Ar laser. The oxime acrylates underwent concomitant photobleaching with initiation of polymerization Application to stereolithog. was discussed.

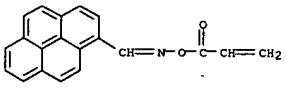
ACCESSION NUMBER: 1991:450446 CAPLUS
DOCUMENT NUMBER: 115:50446
TITLE: Laser-induced three-dimensional photopolymerization using visible initiators and UV cross-linking by photosensitive comonomers
AUTHOR(S): Kumar, G. Sudesh; Neckers, D. C.
CORPORATE SOURCE: Cent. Photochem. Sci., Bowling Green State Univ., Bowling Green, OH, 43403, USA
SOURCE: Macromolecules (1991), 24(15), 4322-7
CODEN: MAMOBX; ISSN: 0024-9297
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **133872-58-9P 133872-59-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and UV crosslinking of)

RN 133872-58-9 CAPLUS
CN 2-Propenoic acid, 1,6-hexanediyl ester, polymer with 1-pyrenecarboxaldehyde O-(1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)

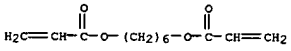
CM 1

CRN 133872-54-5
CMF C20 H13 N O2



CM 2

CRN 13048-33-4
CMF C12 H18 O4

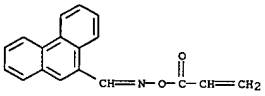


RN 133872-59-0 CAPLUS
CN 2-Propenoic acid, 1,6-hexanediyl ester, polymer with 9-phenanthrenecarboxaldehyde O-(1-oxo-2-propenyl)oxime (9CI) (CA INDEX

L19 ANSWER 14 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
NAME)

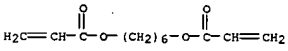
CM 1

CRN 133872-55-6
CMF C18 H13 N O2



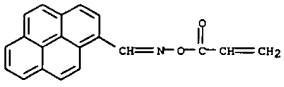
CM 2

CRN 13048-33-4
CMF C12 H18 O4

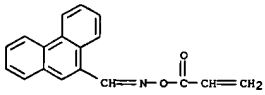


IT **133872-54-5P 133872-55-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and spectral characteristics and photopolymerizability of)

RN 133872-54-5 CAPLUS
CN 1-Pyrenecarboxaldehyde, O-(1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)



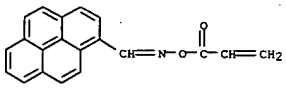
RN 133872-55-6 CAPLUS
CN 9-Phenanthrenecarboxaldehyde, O-(1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)



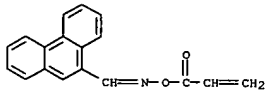
IT **133872-54-5DP**, polymers with bisphenol diacrylates
133872-55-6DP, polymers with bisphenol diacrylates

L19 ANSWER 14 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, eosin-sensitized laser)

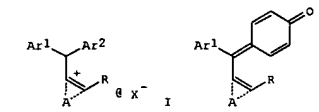
RN 133872-54-5 CAPLUS
CN 1-Pyrenecarboxaldehyde, O-(1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)



RN 133872-55-6 CAPLUS
CN 9-Phenanthrenecarboxaldehyde, O-(1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)

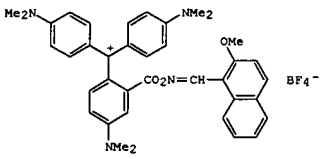


L19 ANSWER 15 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
GI



I

II



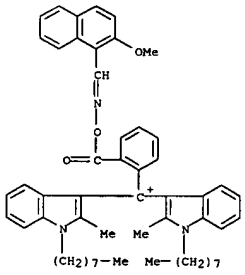
III

AB The title photohardenable composition comprises ≥1 dye from I and II [Ar1, Ar2 = aryl, heterocyclyl; R = CO2N:CR1R2, CO2CR3R4CR5R6Y; R1-R 6 = H, alkyl, aralkyl, aryl, heteroaryl; R1 and R2 = H at the same time; Y = CN, NO2, SO2R7, SOR7, COR7, CO2R7, CONR7R8; R7, R8 = R1; A = 5- or 6-membered ring; X = anion; the group C6H4-p-O in II may be condensed with
an arom or heterocyclic ring], e.g., III. The above dye acts as spectral sensitizer for photopolymn. initiator in the composition The composition has
improved sensitivity.

ACCESSION NUMBER: 1991:72335 CAPLUS
DOCUMENT NUMBER: 114:72335
TITLE: Light- and heat-sensitive compositions, and recording material and method using them
INVENTOR(S): Yamaguchi, Jun; Ishige, Sadao; Washizu, Shintaro; Itoh, Isamu; Sato, Kozo
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Ger. Offen., 19 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4001363	A1	19900719	DE 1990-4001363	19900118
JP 02289856	A2	19901129	JP 1989-314975	19891204
US 5180652	A	19930119	US 1990-466906	19900118
PRIORITY APPLN. INFO.:			JP 1989-9509 A	19890118
			JP 1989-314975 A	19891204

L19 ANSWER 15 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CMF C54 H62 N3 O3



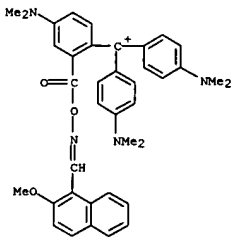
CM 2

CRN 14874-70-5
CMF B F4
CCI CCS

L19 ANSWER 15 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
OTHER SOURCE(S): MARPAT 114:72335
IT **131420-01-4P 131923-27-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and use of, as spectral sensitizer for photopolymn. catalysts)
RN 131420-01-4 CAPLUS
CN Methylium, [4-(dimethylamino)-2-[[[[(2-methoxy-1-naphthalenyl)methylene]amino]oxy]carbonyl]phenyl]bis[4-(dimethylamino)phenyl]-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 131420-00-3
CMF C38 H39 N4 O3



CM 2

CRN 14874-70-5
CMF B F4
CCI CCS

RN 131923-27-8 CAPLUS
CN Methylium, [2-[[[[(2-methoxy-1-naphthalenyl)methylene]amino]oxy]carbonyl]phenyl]bis(2-methyl-1-octyl-1H-indol-3-yl)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 131923-26-7

L19 ANSWER 16 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
GI For diagram(s), see printed CA Issue.
AB The title materials contain a thermally decolorizable dye I or II [R, R1 =
aryl, heteroaryl, R and R1 may form a ring; R2 = alkyl, alkenyl, aralkyl, aryl, heteroaryl; A = 5- or 6-membered ring; (all the groups, rings, and the benzoquinone ring of II may be substituted; X- = monovalent anion). The materials provide decolored images on heating. Thus, a poly(ethylene terephthalate) film was coated with a heat-sensitive layer containing III to
give a blue thermal recording film.

ACCESSION NUMBER: 1991:52979 CAPLUS
DOCUMENT NUMBER: 114:52979
TITLE: Recording materials using thermally decolorizable dyes
INVENTOR(S): Sato, Kozo
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

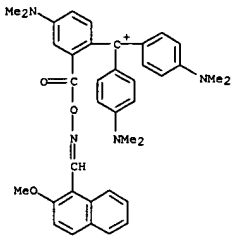
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02164590	A2	19900625	JP 1988-320164	19881219
JP 07084104	B4	19950913		
US 4981833	A	19910101	US 1989-452650	19891219
PRIORITY APPLN. INFO.:			JP 1988-320164 A	19881219

IT **131420-01-4P**
RL: PREP (Preparation)
(preparation of, thermally decolorizable dye, thermal recording material
using)
RN 131420-01-4 CAPLUS
CN Methylium, [4-(dimethylamino)-2-[[[[(2-methoxy-1-naphthalenyl)methylene]amino]oxy]carbonyl]phenyl]bis[4-(dimethylamino)phenyl]-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 131420-00-3
CMF C38 H39 N4 O3

L19 ANSWER 16 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



CM 2

CRN 14874-70-5
CMF B F4
CCI CCS

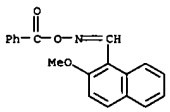
L19 ANSWER 17 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

AB In the title photog. material with ≥1 unfogged internal latent image-type Ag halide emulsion layer and a back layer on the other side of the emulsion layer, the back layer contains an acid precursor and/or acid polymer.

ACCESSION NUMBER: 1990:581274 CAPLUS
DOCUMENT NUMBER: 113:181274
TITLE: Direct positive photographic material
INVENTOR(S): Inoue, Akiyuki; Okamura, Hisashi
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 25 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02056544	A2	19900226	JP 1989-70162	19890322
PRIORITY APPLN. INFO.:			JP 1988-115640	A1 19880512

IT **99806-90-3**
RL: USES (Uses)
(acid precursor, back layer containing, for direct pos. photog. material)
RN 99806-90-3 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-benzoyloxime (9CI) (CA INDEX NAME)



L19 ANSWER 18 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

GI For diagram(s), see printed CA Issue.

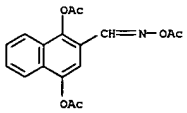
AB The title compds. [I; R1, R4 = H, acyl, alkoxycarbonyl, alkylsulfonyl, dialkylcarbamoyl, alkoxyalkyl, alkyl; R2 = cyano, CHO, N-acyloxyiminomethyl, substituted CONH2, acylalkyl, (CH2CH:CMeCH2)nH (n = 2-4), CH2CH:CMe2, acyloxyalkyl, alkoxycarbonylalkyl, (un)substituted alkylsulfonyl, SO3H, substituted OH or NH2, N-substituted CH2NH2, CO2H, R; R3 = H, alkyl, acyloxyalkyl, etc.], useful for wound healing and for treatment of delayed allergies, are prepared Thus, treatment of 1,4-naphthalenediol ditetrahydropyranyl ether (preparation given) with BuLi in Et2O followed by DMF gave, after deprotection, 2-formyl-1,4-dihydroxynaphthalene which was acetylated with Ac2O in pyridine to give 2-formyl-1,4-diacetoxynaphthalene. I inhibited 24.2-96.6% auricle edema in mice sensitized with oxazolone.

ACCESSION NUMBER: 1990:118481 CAPLUS
DOCUMENT NUMBER: 112:118481
TITLE: Preparation of 1,4-dihydroxynaphthalene derivatives for wound healing and for treatment of delayed allergies
INVENTOR(S): Imuda, Junichi; Ishitoku, Takeshi; Isayama, Shigeru; Furuya, Yoshiro; Takahashi, Katsuya; Ori, Aiichiro; Nakamura, Hideo; Motoyoshi, Satoru
PATENT ASSIGNEE(S): Mitsui Petrochemical Industries, Ltd., Japan; Dainippon Pharmaceutical Co., Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 47 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01203351	A2	19890816	JP 1988-25330	19880205
PRIORITY APPLN. INFO.:			JP 1988-25330	19880205

OTHER SOURCE(S): MARPAT 112:118481

IT **125499-32-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as allergy inhibitor and for wound healing)
RN 125499-32-3 CAPLUS
CN 2-Naphthalenecarboxaldehyde, 1,4-bis(acetyloxy)-, 2-(O-acetyloxime) (9CI) (CA INDEX NAME)



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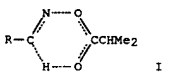
GI

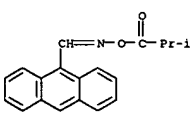


I

AB Decrease in the thermolysis rate constant of RCH:NO2CCHMe2 (R = 9-anthryl) with increasing solvent polarity, solvent independence of ΔH.thermod. and ΔS.thermod., and the neg value of ΔS.thermod. were all attributed to a mechanism involving a cyclic transition state (I).

ACCESSION NUMBER: 1989:438728 CAPLUS
DOCUMENT NUMBER: 111:38728
TITLE: Kinetics and mechanism of thermolysis of 9-formylanthracene oxime isobutyrate
AUTHOR(S): Lazareva, A. M.; Stankevich, A. I.
CORPORATE SOURCE: Beloruss. Gos. Univ., Minsk, USSR
SOURCE: Kinetika i Kataliz (1988), 29(5), 1248
CODEN: KNKTA4; ISSN: 0453-8811
DOCUMENT TYPE: Journal
LANGUAGE: Russian

IT **120625-63-0**, 9-Formylanthracene oxime isobutyrate
RL: RCT (Reactant); RACT (Reactant or reagent)
(thermal decomposition of, kinetics and mechanism of)
RN 120625-63-0 CAPLUS
CN 9-Anthracenecarboxaldehyde, O-(2-methyl-1-oxopropyl)oxime (9CI) (CA INDEX NAME)



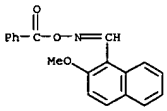
L19 ANSWER 20 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

AB A photothermog. material has ≥1 shielding layers which temporarily shield acid activity. The shielding layers may contain a fusible agent or a substance which is dissolved in or expanded with the fusible agent under heat-developing temperature The photothermog. material shows improved heat-developing stability and storage stability.

ACCESSION NUMBER: 1988:501932 CAPLUS
DOCUMENT NUMBER: 109:101932
TITLE: Photothermographic material with improved heat-developing stability and storage stability
INVENTOR(S): Goto, Sohei; Komamura, Tawara; Kono, Junichi
PATENT ASSIGNEE(S): Konica Co., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 45 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63004233	A2	19880109	JP 1986-147284	19860624
JP 08012412	B4	19960207		
PRIORITY APPLN. INFO.:			JP 1986-147284	19860624

IT **99806-90-3**
RL: USES (Uses)
(acid precursor, fusible agent containing, for photothermog. material)
RN 99806-90-3 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-benzoyloxime (9CI) (CA INDEX NAME)



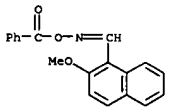
L19 ANSWER 21 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

AB A photothermog. material comprising a support, photosensitive Ag halide, color-formers, a reducing agent, a binder, and microcapsules is claimed wherein the microcapsule core material contains an acid and/or an acid-precursor. The material retains high contrast even after prolonged storage.

ACCESSION NUMBER: 1988:430203 CAPLUS
DOCUMENT NUMBER: 109:30203
TITLE: Photothermographic material containing microencapsulated acid(-precursor) for improved storage stability
INVENTOR(S): Okauchi, Ken; Kakuchi, Hiroyuki; Yamazaki, Hiroshi
PATENT ASSIGNEE(S): Konica Co., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 45 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62288837	A2	19871215	JP 1986-132473	19860607
JP 05079977	B4	19931105		
PRIORITY APPLN. INFO.:			JP 1986-132473	19860607

IT **99806-90-3**
RL: USES (Uses)
(photothermog. material containing microcapsules of, for improved storage stability)
RN 99806-90-3 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-benzoyloxime (9CI) (CA INDEX NAME)



L19 ANSWER 22 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

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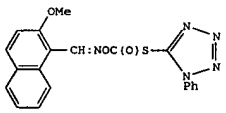


I

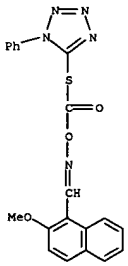
AB A Ag halide photog. material having ≥1 light-sensitive Ag halide emulsion layer contains ≥1 photog. reagent precursor of the formula R1CH:NOCY(LX)mTn(PUG) (R1 = H, other monovalent substituent; Y = O, NR2; R2 = substituent; L = bivalent linkage group; X = electron-attracting center; T = timing group; PUG = photog. useful group having O, N or cyclic structure; n, m = 0, 1). The precursor, which is quite stable during storage of the material, releases the photog. reagent at an appropriate time during its development. It is especially useful for development at low pH, e.g. 9-12, and for dry thermal processing. Thus, development inhibitor precursor I was added to the emulsion layer of an exptl. monocolor photog. film as a coupler/precursor codispersion. Upon exposure and then development by a normal color neg. process, it produced a remarkable reduction in fog without affecting speed or contrast.

ACCESSION NUMBER: 1988:177038 CAPLUS
DOCUMENT NUMBER: 108:177038
TITLE: Timing precursor in silver halide photographic material
INVENTOR(S): Ito, Isamu; Kawada, Ken
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62163051	A2	19870718	JP 1986-4290	19860114
JP 07062757	B4	19950705		
PRIORITY APPLN. INFO.:			JP 1986-4290	19860114

IT **114040-46-9P**
RL: PREP (Preparation)
(preparation of, as timing photog. development inhibitor precursor)
RN 114040-46-9 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-[[(1-phenyl-1H-tetrazol-5-yl)thio]carbonyl]oxime (9CI) (CA INDEX NAME)

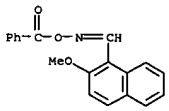
L19 ANSWER 22 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L19 ANSWER 23 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
AB The title photothermog. photosensitive materials contain a photosensitive Ag halide, a reducing agent, a binder, and an acid (or its precursor) which is dispersed (as particles) together with a thermoplastic polymer. The photothermog. materials give high-contrast images even after the materials are stored for a period of time.
ACCESSION NUMBER: 1988:140810 CAPLUS
DOCUMENT NUMBER: 108:140810
TITLE: Photothermographic photosensitive materials with excellent storage stability and high contrast
INVENTOR(S): Iwagaki, Masaru; Goto, Sohei; Oya, Hidenobu
PATENT ASSIGNEE(S): Konica Co., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 51 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62240962	A2	19871021	JP 1986-85587	19860414
JP 06082210	B4	19941019		
PRIORITY APPLN. INFO.:			JP 1986-85587	19860414

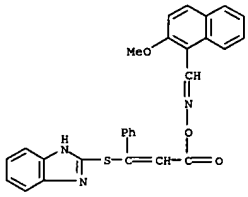
IT **99806-90-3**
RL: USES (Uses)
(photothermog. materials containing, storage stability improvement of)
RN 99806-90-3 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-benzoyloxime (9CI) (CA INDEX NAME)



L19 ANSWER 24 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
AB In the title process, the heating of imaging materials is carried out in the presence of the compound of the formula R1CX:CR2CO2N:CHR3 (R1, R2 = H, alkyl, cycloalkyl, alkenyl, alkynyl, aralkyl, aryl, heterocyclyl, carboxyl or its salt, halo, CN, alkylsulfonyl, arylsulfonyl, sulfamoyl, carbamoyl, alkoxycarbonyl, aryloxycarbonyl, alkylphosphoryl, arylphosphoryl, alkylphosphinyl, arylphosphinyl, alkylsulfinyl, arylsulfinyl, acyl, amino, acylamino, acyloxy, photog. useful group, R3 = aryl, heterocyclyl; X = photog. useful group; R1R2 combination may form a ring). The above compds. release development inhibitors with excellent timing.
ACCESSION NUMBER: 1987:415617 CAPLUS
DOCUMENT NUMBER: 107:15617
TITLE: Imaging process involving heating step
INVENTOR(S): Sato, Kozo; Kato, Masatoshi; Kitaguchi, Hiroshi
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 19 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

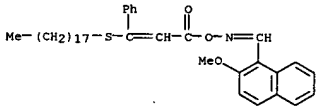
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61267045	A2	19861126	JP 1985-106872	19850521
JP 05033780	B4	19930520		
PRIORITY APPLN. INFO.:			JP 1985-106872	19850521

IT **108831-28-3 108831-29-4 108859-52-5**
RL: USES (Uses)
(photothermog. development inhibitor-releasing compds.)
RN 108831-28-3 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-[3-(1H-benzimidazol-2-ylthio)-1-oxo-3-phenyl-2-propenyl]oxime (9CI) (CA INDEX NAME)

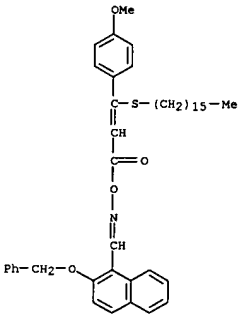


RN 108831-29-4 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-[3-(octadecylthio)-1-oxo-3-phenyl-2-propenyl]oxime (9CI) (CA INDEX NAME)

L19 ANSWER 24 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 108859-52-5 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-(phenylmethoxy)-, O-[3-(hexadecylthio)-3-(4-methoxyphenyl)-1-oxo-2-propenyl]oxime (9CI) (CA INDEX NAME)



IT **108831-27-2P**
RL: PREP (Preparation)
(preparation of, as photothermog. development inhibitor releasing compound)
RN 108831-27-2 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-[3-[[4-(dodecyloxy)phenyl]thio]-1-oxo-3-phenyl-2-propenyl]oxime (9CI) (CA INDEX NAME)

L19 ANSWER 24 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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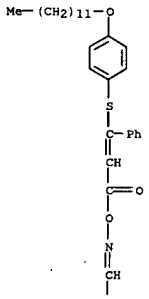
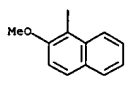


PAGE 2-A



L19 ANSWER 25 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
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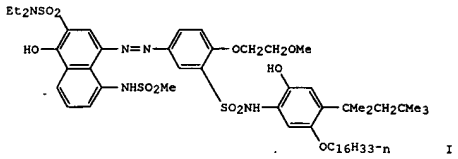
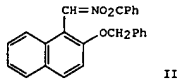


I



II

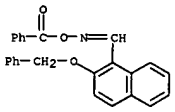
AB The claimed photothermog. photosensitive materials contain internal latent
image type Ag halide emulsions, nucleation agents, organic Ag salt type oxidizing agent, and a base or its precursor which releases the base upon heating. The photothermog. material give high contrast pos. images. Thus, an internal latent image type Ag(Br,I) emulsion, a benzotriazole Ag emulsion, PhNHCSNH-m-C6H4CONH-p-C6H4NHNHCHO, a dispersion of I, a p-C9H19C6H4O(CH2CH2O)10H solution, a H2NSO2NMe2 solution, guanidine trichloroacetate, and a dispersion of II were mixed, then the mixture was coated on a film support to give a photothermog. photosensitive material which gave pos. image with high Dmax and low Dmin.

ACCESSION NUMBER: 1986:616732 CAPLUS
DOCUMENT NUMBER: 105:216732
TITLE: Photothermographic photosensitive materials
INVENTOR(S): Hara, Hiroshi; Daimatsu, Hideki
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 33 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

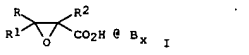
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61107243	A2	19860526	JP 1984-228550	19841030
PRIORITY APPLN. INFO.:			JP 1984-228550	19841030

IT **100906-56-7**
RL: USES (Uses)
(direct pos. photothermog. photosensitive materials containing)
RN 100906-56-7 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-(phenylmethoxy)-, O-benzoyloxime (9CI) (CA

L19 ANSWER 25 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
INDEX NAME)



L19 ANSWER 26 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
GI



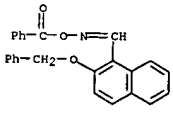
I

AB The claimed photothermog. photosensitive materials contain a compound of the
formula I (R, R1 = H, alkyl, cycloalkyl, alkenyl, alkynyl, aryl, heterocyclyl, aralkyl, CO2M; RR1 in combination may form a ring; R2 = H, alkyl, cycloalkyl, alkenyl, aryl, alkynyl, heterocyclyl, aralkyl; M = H, alkali metal, H.Bx; B = an organic base; x = 1 when B is a monoacidic base,
and x = 1/2 when B is a diacidic base). The compound I shows good storage
stability and excellent base-releasing property.

ACCESSION NUMBER: 1986:616726 CAPLUS
DOCUMENT NUMBER: 105:216726
TITLE: Thermal development type photosensitive imaging materials
INVENTOR(S): Kawada, Ken; Yabuki, Yoshiharu; Sato, Kozo; Hirai, Hiroyuki
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 28 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61053635	A2	19860317	JP 1984-176397	19840824
JP 05054643	B4	19930813		
US 4619888	A	19861028	US 1985-769297	19850826
PRIORITY APPLN. INFO.:			JP 1984-176397 A	19840824

IT **100906-56-7**
RL: USES (Uses)
(photothermog. materials containing, base precursors for)
RN 100906-56-7 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-(phenylmethoxy)-, O-benzoyloxime (9CI) (CA
INDEX NAME)



L19 ANSWER 26 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

L19 ANSWER 27 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

AB The claimed photothermog. photosensitive materials contain a base precursor of the formula [RpZ(O)qNR1CR2R3CO2H]n.Xm [Z = C, N, S; R, R1 = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, alkoxy, aryloxy, alkylthio, arylthio, heterocyclyl, acyl; R2, R3 = H, halo, alkyl, alkenyl, alkynyl, cycloalkyl, aralkyl, aryl, alkoxy, aryloxy, alkythio, arythio, heterocyclyl, acylamino, alkylsulfinyl, arylsulfinyl, nitro, acyl, sulfamoyl, carbamoyl, alkoxycarbonyl, aryloxycarbonyl, CO2H.X, R42P(O), OH; R4 = alkyl, aryl, aryloxy, alkoxy; X = a base; n, m = 1, 2; p = 0, 1; q = 1, 2]. The photothermog. materials have good storage stability and thermal development characteristics.

ACCESSION NUMBER: 1986:600549 CAPLUS
DOCUMENT NUMBER: 105:200549
TITLE: Photothermographic photosensitive materials
INVENTOR(S): Yabuki, Yoshiharu; Sato, Kozo; Kawada, Ken; Hirai, Hiroyuki
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

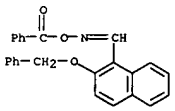
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61055645	A2	19860320	JP 1984-176999	19840825
US 4649103	A	19870310	US 1985-769299	19850826

PRIORITY APPLN. INFO.: JP 1984-176999 A 19840825

OTHER SOURCE(S): CASREACT 105:200549

IT **100906-56-7**
RL: USES (Uses)
(photothermog. photosensitive materials containing, base precursor for)

RN 100906-56-7 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-(phenylmethoxy)-, O-benzoyloxime (9CI) (CA INDEX NAME)



L19 ANSWER 28 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

AB The claimed material has on the same support having the photothermog. Ag halide emulsion layer or on a different support an elec. conductive layer.
The above elec. conductive layer contains at least: (1) an elec. conductivity-providing substance, (2) a compound having m.p. >100°, and (3)
a hydrophilic binder. The above elec. conductive layer may contain C black, propylurea, and gelatin.

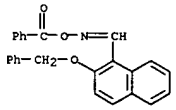
ACCESSION NUMBER: 1986:470171 CAPLUS
DOCUMENT NUMBER: 105:70171
TITLE: Silver halide photothermographic material
INVENTOR(S): Sawada, Satoru; Naito, Hideki; Kitaguchi, Hiroshi
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 18 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61029835	A2	19860210	JP 1984-151815	19840720
US 4643964	A	19870217	US 1985-757556	19850722

PRIORITY APPLN. INFO.: JP 1984-151815 A 19840720

IT **100906-56-7**
RL: USES (Uses)
(silver halide photothermog. materials with elec. conductive layer containing)

RN 100906-56-7 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-(phenylmethoxy)-, O-benzoyloxime (9CI) (CA INDEX NAME)



L19 ANSWER 29 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

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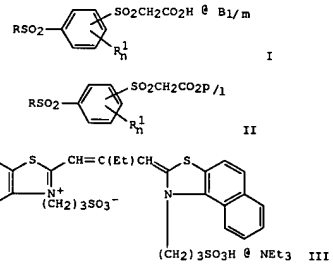


AB A heat-developable color photog. composition is comprised of a photog. coupler,
Ag halides, ≥1 base precursor having the formula I or II [R = alkyl, cycloalkyl, alkenyl, alkynyl, aryl or heterocyclyc; R1 = organic substituent; B = monoacidic or diacidic base; M = alkali or alkaline earth
metal; l = valence of M; m = 1, 2; n = 0-4), and optionally an organic acid
Ag salt. The photog. composition provides images of high d. and less fog over
a short developing time and is excellent in stability. Thus, a Ag(Br,I)-gelatin emulsion, a dispersion of the cyan coupler III in gelatin, a solution of the base precursor CH3SO2-p-C6H4SO2CH2CO2H·HN=C(NH2)2, a gelatin solution, and an aqueous 2,6-dichloro-p-aminophenol solution were mixed, coated on a poly(ethylene terephthalate) film, dried, imagewise exposed to a W lamp (2000 lx) for 5 s, and heated uniformly on a heat block (150°) for 20 s to provide a neg. cyan dye image having Dmax 2.13 and Dmin 0.26.

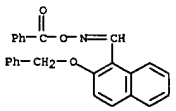
ACCESSION NUMBER: 1986:216386 CAPLUS
DOCUMENT NUMBER: 104:216386
TITLE: Heat developable light-sensitive material
INVENTOR(S): Yabuki, Yoshiharu; Kawata, Ken; Hirai, Hiroyuki
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd. , Japan
SOURCE: Eur. Pat. Appl., 71 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 160996	A2	19851113	EP 1985-105700	19850509
EP 160996	A3	19861120		
EP 160996	B1	19881123		
R: DE, GB, NL				
JP 60237443	A2	19851126	JP 1984-92558	19840509
JP 04013703	B4	19920310		

PRIORITY APPLN. INFO.: JP 1984-92558 A 19840509

IT **100906-56-7**
RL: USES (Uses)
(heat-developable photog. materials containing, alkylsulfonylphenylsulfonylacetic acid base precursor for)

RN 100906-56-7 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-(phenylmethoxy)-, O-benzoyloxime (9CI) (CA INDEX NAME)



L19 ANSWER 30 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
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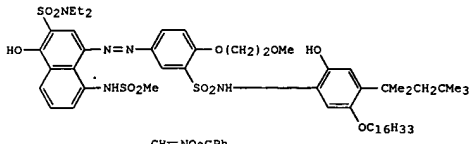
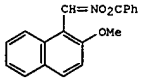


I



II

AB Heat-developable photosensitive materials giving an image with a high signal-to-noise ratio, that is a high Dmax and a low Dmin, and a high d. are composed of a photosensitive gelatin-Ag halide emulsion layer, a dye-forming substance that upon reduction at a high temperature produces a diffusible dye, and an organic acid precursor with the structural unit -CH:NO2C- that is very stable at .ltorsim.50°, but frees an acid at temps. proceeding to development to neutralize the base and stop the development. Thus, a PET support was coated with a composition containing a gelatin-Ag(Br,I) emulsion 20, a gelatin-Ag benzotriazole emulsion 10, a dispersion of I 33 g, a 5% aqueous solution of p-C9H19C6H4O(CH2CH2O)10H 10, a 10% aqueous solution of H2NSO2NMe2 4, a gelatin dispersion of II 10 mL, and a solution of guanidine trichloroacetate 1.6 mL in EtOH 16 mL at 33μ (wet). After drying a gelatin protective layer was added. The resultant material was then imagewise exposed 10 s at 2000 lx with a W lamp, heated for 60 s on a 140° heating block, contacted with a wet receptor sheet, and heated 6 s at 80° to give a Dmax of 2.10 and a Dmin of 0.20 vs. 2.35 and 0.85, resp., for a II-free control.

ACCESSION NUMBER: 1986:139353 CAPLUS
DOCUMENT NUMBER: 104:139353
TITLE: Heat-developing light-sensitive color material
INVENTOR(S): Kato, Masatoshi; Kitaguchi, Hiroshi
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd. , Japan
SOURCE: Ger. Offen., 90 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

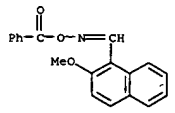
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3508761	A1	19850919	DE 1985-3508761	19850312
JP 60192939	A2	19851001	JP 1984-48305	19840314
JP 04069775	B4	19921109		
US 4656126	A	19870407	US 1985-711885	19850314

PRIORITY APPLN. INFO.: JP 1984-48305 A 19840314

L19 ANSWER 30 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

IT **99806-90-3 99806-94-7 100906-55-6 100906-56-7 100906-57-8**
RL: USES (Uses)
(color diffusion-transfer photothermog. materials containing base-neutralizing acid precursor from, for improved image quality)

RN 99806-90-3 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-benzoyloxime (9CI) (CA INDEX NAME)



RN 99806-94-7 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O,O'-(1,4-phenylenedicarbonyl)dioxime (9CI) (CA INDEX NAME)

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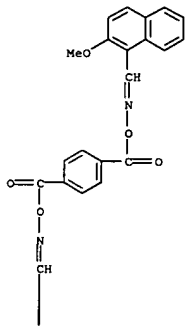

L19 ANSWER 30 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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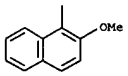
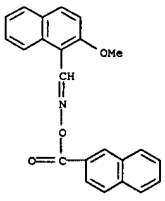
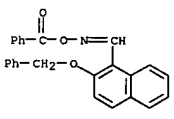


RN 100906-55-6 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-(2-naphthalenylcarbonyl)oxime (9CI) (CA INDEX NAME)

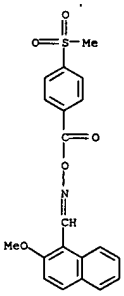


RN 100906-56-7 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-(phenylmethoxy)-, O-benzoyloxime (9CI) (CA INDEX NAME)



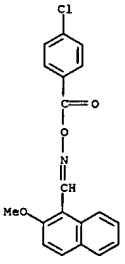
RN 100906-57-8 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-[4-(methylsulfonyl)benzoyl]oxime (9CI) (CA INDEX NAME)

L19 ANSWER 30 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



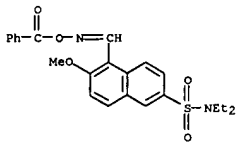
IT **99806-93-6P 100906-58-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and photothermog. applications of, as acid precursor)

RN 99806-93-6 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-(4-chlorobenzoyl)oxime (9CI) (CA INDEX NAME)



RN 100906-58-9 CAPLUS
CN 2-Naphthalenesulfonamide, 5-[[(benzoyloxy)imino]methyl]-N,N-diethyl-6-methoxy- (9CI) (CA INDEX NAME)

L19 ANSWER 30 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L19 ANSWER 31 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

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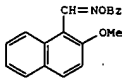


I

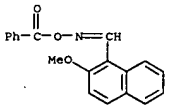
AB Organic acid precursors (R1CH:NO2C)nX [R1 = (un)substituted alkyl, cycloalkyl, aralkyl, alkenyl, (un)substituted aryl, heterocyclyl; X = (un)substituted alkyl, cycloalkyl, aralkyl, (un)substituted aryl, heterocycyl, or a mono-, di-, or trivalent group formed by combination of the above; n = 1-3], useful as agents to end development in a thermal photog. development process, were prepared Thus, 103.2 g 2-hydroxy-1-naphthaldehyde in DMF was etherified with 4-MeC6H4SO3Me and K2CO3 at 50-60° for 2 h to give 93.8 g 2-methoxy-1-naphthaldehyde, which (80 g) underwent oximation to give 85 g oxime. The oxime (70.3 g) was treated with 60% NaH in MeCN, and the resulting solution treated with BzCl at 10° to give 88 g acid precursor I. The reaction rate constant for cleavage of I to BzOH was 2.01/h at 100°, with T1/2 = 0.34 h.

ACCESSION NUMBER: 1986:50692 CAPLUS
DOCUMENT NUMBER: 104:50692
TITLE: Photographic material containing an acid precursor and
a procedure for producing a photographic image
INVENTOR(S): Kitaguchi, Hiroshi; Kato, Masatoshi
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd. , Japan
SOURCE: Ger. Offen., 40 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

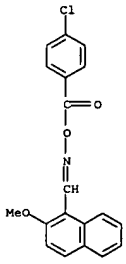
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3442018	A1	19850530	DE 1984-3442018	19841116
JP 60108837	A2	19850614	JP 1983-216928	19831117
US 4670373	A	19870602	US 1984-672643	19841119
PRIORITY APPLN. INFO.:			JP 1983-216928 A	19831117

IT **99806-90-3P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and decomposition kinetics of)
RN 99806-90-3 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-benzoyloxime (9CI) (CA INDEX NAME)

L19 ANSWER 31 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



IT **99806-93-6P 99806-94-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as acid precursor for photog. emulsions)
RN 99806-93-6 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O-(4-chlorobenzoyl)oxime (9CI) (CA INDEX NAME)



RN 99806-94-7 CAPLUS
CN 1-Naphthalenecarboxaldehyde, 2-methoxy-, O,O'-(1,4-phenylenedicarbonyl)dioxime (9CI) (CA INDEX NAME)

L19 ANSWER 31 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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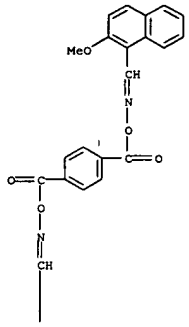

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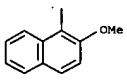

L19 ANSWER 32 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
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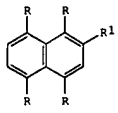


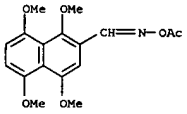
I

AB Alkoxynaphthalenes and their salts I [R = alkoxy; R1 = HOCH2, halomethyl, R2ON:CH (where R2 = H, alkyl), (CR3H)nR4 (where R3 = H, alkyl and R4 = CO2H, alkoxycarbonyl, cyano; n = 0, 1)], having inflammation inhibiting, antihypertensive, analgesic, antiallergic, and antihistaminic activities (no data), were prepared Thus, aqueous NaOH was added dropwise to a suspension of 1.8 g I (R = OMe; R1 = CHO) and 2.2 g Ag2O in CH2Cl2 and the resulting mixture heated 24 h at 60° to give 1 g I (R = OMe; R1 = CO2H).

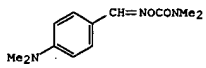
ACCESSION NUMBER: 1985:471078 CAPLUS
DOCUMENT NUMBER: 103:71078
TITLE: Alkoxynaphthalene derivatives
PATENT ASSIGNEE(S): Otsuka Pharmaceutical Factory, Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 60036434	A2	19850225	JP 1983-145447	19830808
JP 03026177	B4	19910410		
PRIORITY APPLN. INFO.:			JP 1983-145447	19830808

OTHER SOURCE(S): CASREACT 103:71078
IT **97476-16-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 97476-16-9 CAPLUS
CN 2-Naphthalenecarboxaldehyde, 1,4,5,8-tetramethoxy-, O-acetyloxime (9CI) (CA INDEX NAME)



L19 ANSWER 33 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
GI



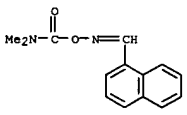
I

AB Photothermog. materials contain in a binder microparticles of a base-releasing precursor which is substantially insol. in water. The materials have good preservation stability due to the precursor having high resistance against self-decomposition by ambient moisture. Thus, a water-insol. type precursor I was mixed with poly(ethylene glycol), gelatin, and water and crushed using a mill to give a dispersion of precursor grains with an average size of 1 μm. The dispersion was then coated on a poly(ethylene terephthalate) support together with a Ag(Br,I) emulsion, a cyan coupler dispersion containing 2-dodecylcarbamoyl-1-naphthol, and 2,6-dichloro-p-aminophenol to form a photosensitive film. The film was imagewise-exposed and heat-developed at 150° for 20 s to give a neg. cyan dye image with Dmax 2.08 and Dmin 0.25.

ACCESSION NUMBER: 1985:123151 CAPLUS
DOCUMENT NUMBER: 102:123151
TITLE: Photothermographic materials
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 59174830	A2	19841003	JP 1983-50000	19830325
JP 03058498	B4	19910905		
US 4514493	A	19850430	US 1984-592197	19840322
PRIORITY APPLN. INFO.:			JP 1983-50000 A	19830325

IT **95186-86-0**
RL: USES (Uses)
(color photothermog. material containing)
RN 95186-86-0 CAPLUS
CN 1-Naphthalenecarboxaldehyde, O-[(dimethylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



L19 ANSWER 33 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

L19 ANSWER 34 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
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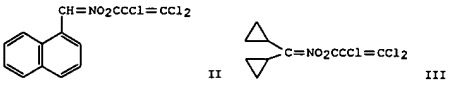


II III

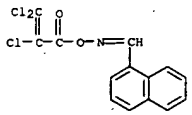
AB Cl2C:CClCO2N:CRR1 (I) (R,R1 = H, lower alkyl, benzyl, cycloalkyl, naphthyl, aryl, etc.) were prepared and shown, in some cases, to be more effective fungicides than kilazin P. Thus, 100 mL PhMe solution containing 40 g Cl2C:CClCOCl were added at ≤20° to 30 g PhCH:NOH and 26 g Et3N in 400 mL PhMe, and the mixture was heated 2 h at 50° to give 58 g I (R = Ph, R1 = H). Among 39 other I prepared were I [R,R1 = Me,Me; Me,Et; (RR1=) cyclohexylidene], the naphthyl analog II, and the dicyclopropyl analog III.

ACCESSION NUMBER: 1984:610740 CAPLUS
DOCUMENT NUMBER: 101:210740
TITLE: Trichloroacryloyl oxime derivatives
INVENTOR(S): Yamada, Yasuo; Saito, Junichi; Gotoh, Toshio; Katsumata, Osamu; Sakawa, Shinji
PATENT ASSIGNEE(S): Nihon Tokushu Noyaku Seizo K. K. , Japan
SOURCE: Eur. Pat. Appl., 34 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 112524	A1	19840704	EP 1983-112276	19831207
EP 112524	B1	19860528		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL				
JP 59110665	A2	19840626	JP 1982-220165	19821217
US 4581365	A	19860408	US 1983-557688	19831202
IL 70443	A1	19870130	IL 1983-70443	19831214
BR 8306913	A	19840724	BR 1983-6913	19831215
ZA 8309329	A	19840829	ZA 1983-9329	19831215
DK 8305810	A	19840618	DK 1983-5810	19831216
AU 8322504	A1	19840621	AU 1983-22504	19831219
PRIORITY APPLN. INFO.:			JP 1982-220165 A	19821217

OTHER SOURCE(S): CASREACT 101:210740
IT **93033-49-9P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as fungicide)
RN 93033-49-9 CAPLUS
CN 1-Naphthalenecarboxaldehyde, O-(2,3,3-trichloro-1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)

L19 ANSWER 34 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

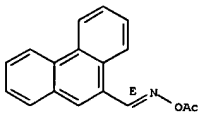


L19 ANSWER 35 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

AB The 70 eV mass spectra of aromatic oxime geometric isomers were measured. Loss of H2O, HO, and HCN were major fragmentations from the mol. ion of the benzaldoximes studied. Halo substituted benzaldoximes eliminated HCNO and H2CNO forming an addnl. fragmentation path from the mol. ion. Three new oxime acetates were prepared and their mass spectra studied.

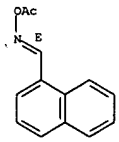
ACCESSION NUMBER: 1974:120070 CAPLUS
DOCUMENT NUMBER: 80:120070
TITLE: Mass spectra of syn- and anti-aromatic aldoximes
AUTHOR(S): Brown, Ellis V.; Hough, Lindsay B.; Plasz, Andrew C.
CORPORATE SOURCE: Dep. Chem., Univ. Kentucky, Lexington, KY, USA
SOURCE: Organic Mass Spectrometry (1973), 7(12), 1337-43
CODEN: ORMSBG; ISSN: 0030-493X
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **51873-99-5 51874-00-1 51874-01-2**
RL: PRP (Properties)
(mass spectrum of)
RN 51873-99-5 CAPLUS
CN 9-Phenanthrenecarboxaldehyde, O-acetyloxime, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 51874-00-1 CAPLUS
CN 1-Naphthalenecarboxaldehyde, O-acetyloxime, (E)- (9CI) (CA INDEX NAME)

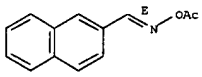
Double bond geometry as shown.



RN 51874-01-2 CAPLUS
CN 2-Naphthalenecarboxaldehyde, O-acetyloxime, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L19 ANSWER 35 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L19 ANSWER 36 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

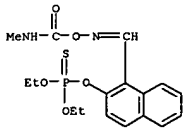
AB The title compds. useful as insecticides, animal systemic parasiticides, herbicides, and foliage fungicides have the formula I. The intermediate 3-(diethoxyphosphinothioyl) benzaldehyde (II), n30D 1.5239 was prepared in 99.5% yield by refluxing 24.4 g. 3-hydroxybenzaldehyde, 37.8 g. O,O-diethylphos-phorochloridothioate, and 16.4 g. K2CO3 in 200 ml. Me Et ketone 4 hrs., the mixture poured into 300 ml. H2O and twice extracted with CHCl3, 7.5 g. Na2CO3.H2O added to a mixture of 27.4 g. II and 7.6 g. hydroxylamine hydrochloride in 300 ml. H2O at room temperature in 20 min., and the mixture stirred one hr. and extracted with C6H6 to give 68.3% 3-(diethoxyphosphinothioyl)benzaldoxime (III), n30D 1.5460. III (10 g.) in 10 ml. acetone was treated with excess MeNCO and poured into 200 ml. C6H6 to give 93.3% 3-(dieth-oxyphosphinothioyl) benzaldoxime methylcarbamate, n30D 1.5394. Similarly prepared in 96.9% yield was 4'-(diethoxyphosphino-thioyl)acetophenone oxime methylcarbamate. A mixture of 56.2 g. 4'-(diethoxyphosphinothioyl)acetophenone, 17.4 g. hydroxylamine hydrochloride, and 4 g. NaOH in 150 ml. 80% EtOH was refluxed 5 min., cooled, and acidified with concentrated HCl to give 93.5% 4'-(diethoxyphosphinothioyl)acetophenone oxime (IV), n30D 1.5393. A mixture of 10.0 g. IV, 3.2 g. AcCl, 4.1 g. Et3N, and 150 ml. C6H6 was refluxed one hr. to give 96.5% 4'-(diethoxy-phosphinothioyl)acetophenone oxime acetate, n30D 1.5279. A solution of 14.5 g. 4-(diethoxyphosphinothioyl)benzaldoxime. (V) in 50 ml. Et2O was added in 30 min. at 10° to 7 g. phosgene in 150 ml. Et2O, the mixture stirred one hr. at 15°, a solution of 17.4 g. morpholine in 10 ml. H2O added at <15°, and the mixture stirred two hrs. at room temperature and worked up to give 89.8% 4-(diethoxy-phosphinothioyl)benzaldoxime 4-morpholinecarboxylate, n30D 1.5423. Similarly 14.5 g. V, 7 g. phosgene, and 8.6 g. N,N-dimethylaniline treated with 6.1 g. ethanolamine and 10 ml. H2O at <15° gave 94.8% 4-(diethoxyphosphinothioyl)benzaldoxime (β-hydroxyethyl)carbamate (VI), n30D 1.5423. A solution of 11.6 g. N,N-diethylethylenediamine in 10 ml. H2O was added dropwise at <15° to VI in Et2O solution to give 51.8% 4-(diethoxyphos-phinothioyl)benzaldoxime 2-(diethylamino)ethyl carbamate, n30D 1.5310. These procedures were followed to obtain the tabulated I (X = S, p = position of phenyl substitution by R2C:NOR3 relative to P-containing group). The following VII were likewise prepared (R, R1, and n30D given): H, CONHMe, 1.5280; H, CONHBu, 1.5130; Me, CONHMe, 1.5243; Me, CONHPr-iso, 1.5109. The compds. prepared were tested as pre- and postemergent herbicides, as foliage fungicides, as insecticides, and for internal animal systematic activity.

ACCESSION NUMBER: 1969:430236 CAPLUS
DOCUMENT NUMBER: 71:30236
TITLE: (O-Carbamoyl oxime), phosphate, phosphonate, and phosphinate compositions and their utility as herbicides and pesticides
INVENTOR(S): Gutman, Arnold D.
PATENT ASSIGNEE(S): Stauffer Chemical Co.
SOURCE: S. African, 80 pp.
CODEN: SFXXAB

L19 ANSWER 36 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

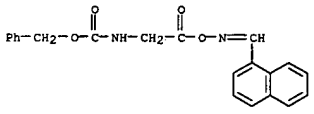
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ZA 6803662		19681108		
DE 1768676			DE	
FR 1583911			FR	
GB 1229853			GB	
US 3652737		19720000	US	
US 3673181		19720000	US	
US 3681476		19720000	US	
US 3681478		19720000	US	
US 3681479		19720000	US	
US 3733375		19730000	US	
US 3749748		19730000	US	
US 3769419		19730000	US	
PRIORITY APPLN. INFO.:			US	19670616
			US	19680520

IT **22942-38-7F**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 22942-38-7 CAPLUS
CN Phosphorothioic acid, O,O-diethyl ester, O-ester with 2-hydroxy-1-naphthaldehyde O-(methylcarbamoyl)oxime (8CI) (CA INDEX NAME)



L19 ANSWER 37 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
AB (Cbo = PhCH2O2C throughout this abstract) Carbobenzoxyglycine (I) reacted with a series of oximes by the anhydride method (A) (Weygand and Steglich, CA 55, 5359b) (average yields 70%) and with Ph2C:CO (method B) (Elmore and Smyth, CA 59, 4033a) (unfavorable results) to give aminoacyl oximes, PhCH2O2CNHCH2CO2N:CRR1, (II), whose rates of aminolysis by PhCH2NH2 were determined in tetrahydrofuran (THF) at 22°. The results were plotted and discussed from the standpoint of substituent effects on carboxyl activation. The new activation method for peptide synthesis was tested with some simple examples. The following standards were prepared from comparative aminolysis: I thiophenyl ester, m. 72°, from I, PhSH, and POCl3 in absolute THF at -15°; I p-nitrophenyl ester, m. 131°. From I, p-O2NC6H4OH, and POCl3 in THF; and I benzyl ester, m. 71°, from equimolar amts. I and PhCH2Cl in boiling dioxane with excess Et3N. Method A. I (20 millimoles) and 20 millimoles absolute Et3N in 20-30 cc. THF treated with 20 millimoles ClCO2Et at -15° with stirring, after 30 min. a solution of the appropriate oxime in THF added, and the mixture stirred 12 hrs. at -15°, kept overnight at room temperature, and worked up (Wieland and Heinke, CA 53, 18880f) gave II. Method B. I (20 millimoles) in THF treated with 20 millimoles Ph2C:CO and 4 cc. M THF-absolute Et3N at -15°, followed after several min. by 20 millimoles appropriate oxime in THF, the solution warmed gradually to room temperature, kept overnight, and worked up, and the product recrystd. from EtOAc-petr. ether or Me2CO-petr. ether gave II. The following II were prepared (R, R1, and m.p. given): Me, Me (III), 110-12°; (RR' =) cyclohexylidene, 80.5-1.5°; H, m-O2NC6H4, 126.5-8.0°; H, p-O2NC6H4, 166.5-7.5°; Me, Ph, 95.5-7.0°; Me, p-tolyl, 104°; Me, p-anisyl, 90°; Ph, Ph (IV), 78-9°; H, α-C10H7 (V), 107-8°; Me, p-BrC6H4, 113-14°, and Me, m-O2NC6H4 (VI), 79-80°. To 10 millimoles I and 10 millimoles absolute Et3N in 30 cc. THF was added 10 millimoles ClCO2Et at -15° with stirring, after 30 min. 10 millimoles appropriate alc. [furfuryl alc., furfuryl mercaptan (VII), or 1-phenyl-3-methyl-5-pyrazolone (VIII)] added, the mixture kept 5 hrs. at room temperature and worked up, and the crude product recrystd. from EtOAc-petr. ether to give I furfuryl ester, m. 70-1°; carbobenzoxyglycyl ester of VII, m. 65-6°; and I 1-phenyl-3-methylpyrazolyl ester (IX) (VIII bound to I as enol ester according to the ir spectrum), m. 131°, resp. EtO2CCH2NH2·HCl (X.HCl) (10 millimoles) suspended in 20 cc. MeCN treated with 10 millimoles absolute Et3N, followed by 10 millimoles III in MeCN, and the mixture kept 24 hrs. at room temperature and worked up gave 61.2% Cbo-Gly-Gly-OEt (XI), m. 81-2°. Similar treatment of 10 millimoles X.HCl in MeCN with 10 millimoles VI, V, and IX gave XI, m. 81-2°, in yields of 73, 85, and 75%, resp. From 50-millimoles amts. L-tyrosine Et ester-HCl (XII.HCl), IV, and absolute Et3N in MeCN was similarly prepared 75% Cbo-Gly-Tyr-OEt (XIII), m. 126-7°, [α]22D 19.1° (c 3, EtOH), and from 50-millimole amts. XII.HCl and IX was similarly prepared 90% XIII, m. 126-7°, [α]22D 19.0° (c 3, EtOH).

L19 ANSWER 37 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
ACCESSION NUMBER: 1965:3302 CAPLUS
DOCUMENT NUMBER: 62:3302
ORIGINAL REFERENCE NO.: 62:631f-h,632a-c
TITLE: N-Protected aminoacyl oximes as new carboxyl-activated compounds for peptide synthesis
AUTHOR(S): Losse, Guenter; Barth, Alfred; Schatz, Karin
CORPORATE SOURCE: Univ. Halle, Germany
SOURCE: Justus Liebigs Annalen der Chemie (1964), 677, 185-90
CODEN: JLACBF; ISSN: 0075-4617
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 62:3302
IT **3249-04-5**, 1-Naphthaldehyde, o-(N-carboxyglycyl)oxime, benzyl ester
(preparation of)
RN 3249-04-5 CAPLUS
CN Carbamic acid, [[[[(1-naphthylmethylene)amino]oxy]carbonyl]methyl]-, benzyl ester (8CI) (CA INDEX NAME)



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DICTIONARY FILE UPDATES:    4 FEB 2005  HIGHEST RN 825667-31-0

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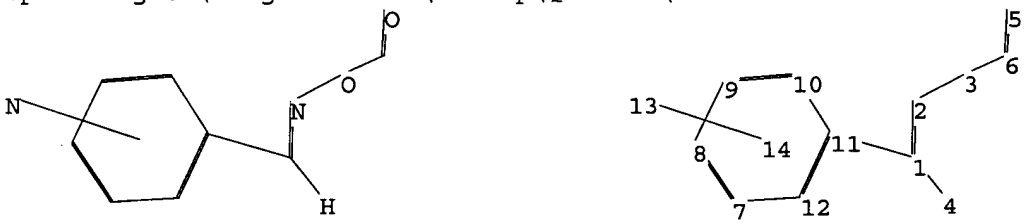


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ring bonds :
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exact bonds :
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normalized bonds :
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Match level :
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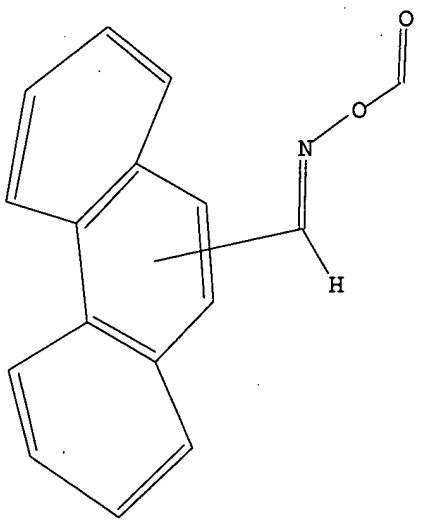

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BATCH **COMPLETE**
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PROJECTED ANSWERS: 0 TO 0

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SEARCH TIME: 00.00.01

L22 3 SEA SSS FUL L20

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)              SINCE FILE      TOTAL
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FILE COVERS 1907 - 6 Feb 2005  VOL 142 ISS 7
FILE LAST UPDATED: 4 Feb 2005  (20050204/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l22
L23           2 L22

=> d l23 1-2 abs ibib hitstr
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L23 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
AB Eosin-sensitized, laser-induced oxime acrylate sensitizer homo- and copolymn. with polyfunctional acrylates followed by UV crosslinking of the acyloxyimino pendent groups was studied. Photopolymerizability of the various oxime acrylates with and without conventional acrylates was determined using an Ar laser. The oxime acrylates underwent concomitant photobleaching with initiation of polymerization Application to stereolithog. was discussed.
ACCESSION NUMBER: 1991:450446 CAPLUS
DOCUMENT NUMBER: 115:50446
TITLE: Laser-induced three-dimensional photopolymerization using visible initiators and UV cross-linking by photosensitive comonomers
AUTHOR(S): Kumar, G. Sudesh; Neckers, D. C.
CORPORATE SOURCE: Cent. Photochem. Sci., Bowling Green State Univ., Bowling Green, OH, 43403, USA
SOURCE: Macromolecules (1991), 24(15), 4322-7
CODEN: MAMOBX; ISSN: 0024-9297
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **133872-59-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and UV crosslinking of)
RN 133872-59-0 CAPLUS
CN 2-Propenoic acid, 1,6-hexanediyl ester, polymer with 9-phenanthrenecarboxaldehyde O-(1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)

CM 1

CRN 133872-55-6
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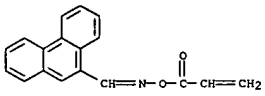

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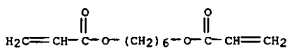
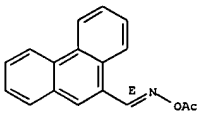


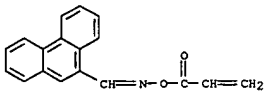
IT **133872-55-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)

L23 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
AB The 70 eV mass spectra of aromatic oxime geometric isomers were measured. Loss of H2O, HO, and HCN were major fragmentations from the mol. ion of the benzaldoximes studied. Halo substituted benzaldoximes eliminated HCNO and H2CNO forming an addnl. fragmentation path from the mol. ion. Three new oxime acetates were prepared and their mass spectra studied.
ACCESSION NUMBER: 1974:120070 CAPLUS
DOCUMENT NUMBER: 80:120070
TITLE: Mass spectra of syn- and anti-aromatic aldoximes
AUTHOR(S): Brown, Ellis V.; Hough, Lindsay B.; Plasz, Andrew C.
CORPORATE SOURCE: Dep. Chem., Univ. Kentucky, Lexington, KY, USA
SOURCE: Organic Mass Spectrometry (1973), 7(12), 1337-43
CODEN: ORMSBG; ISSN: 0030-493X
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **51873-99-5**
RL: PRP (Properties)
(mass spectrum of)
RN 51873-99-5 CAPLUS
CN 9-Phenanthrenecarboxaldehyde, O-acetyloxime, (E)- (9CI) (CA INDEX NAME)

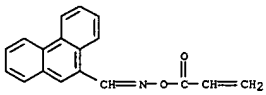
Double bond geometry as shown.



L23 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
(prepn. and spectral characteristics and photopolymerizability of)
RN 133872-55-6 CAPLUS
CN 9-Phenanthrenecarboxaldehyde, O-(1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)



IT **133872-55-6DP**, polymers with bisphenol diacrylates
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, eosin-sensitized laser)
RN 133872-55-6 CAPLUS
CN 9-Phenanthrenecarboxaldehyde, O-(1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)



=> fil reg
COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 10.33 | 1717.17

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION
CA SUBSCRIBER PRICE | -1.46 | -50.27

FILE 'REGISTRY' ENTERED AT 15:41:33 ON 06 FEB 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 4 FEB 2005 HIGHEST RN 825667-31-0
DICTIONARY FILE UPDATES: 4 FEB 2005 HIGHEST RN 825667-31-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

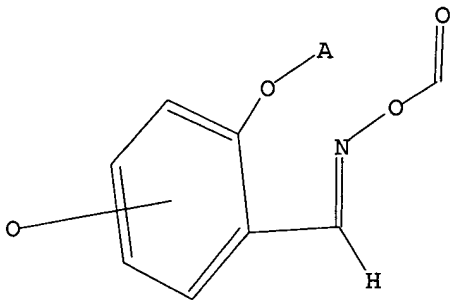
=>
Uploading C:\Program Files\Stnexp\Queries\09734625.str

chain nodes :
1 2 3 4 5 6 13
ring nodes :
7 8 9 10 11 12
chain bonds :
1-2 1-4 1-11 2-3 3-6 5-6
ring bonds :
7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-2 2-3 3-6 5-6
exact bonds :
1-4 1-11
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS

L24 STRUCTURE UPLOADED

=> d query
L24 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l24
SAMPLE SEARCH INITIATED 15:45:56 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 97 TO ITERATE

100.0% PROCESSED 97 ITERATIONS 8 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1350 TO 2530
PROJECTED ANSWERS: 8 TO 329

L25 8 SEA SSS SAM L24

=> s l24 full
FULL SEARCH INITIATED 15:46:01 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1565 TO ITERATE

100.0% PROCESSED 1565 ITERATIONS 177 ANSWERS
SEARCH TIME: 00.00.01

L26 177 SEA SSS FUL L24

=> fil caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	164.34	1881.51

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-50.27

FILE 'CAPLUS' ENTERED AT 15:46:06 ON 06 FEB 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 6 Feb 2005 VOL 142 ISS 7
FILE LAST UPDATED: 4 Feb 2005 (20050204/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l26
L27 30 L26

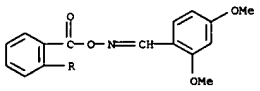
=> d l27 1-30 abs ibib hitstr

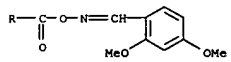
L27 ANSWER 1 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN
AB The title printing plate master contains a photothermal conversion material, a phenolic alkaline-soluble resin, and an organic acid precursor having a structure of -CH:NOCO- or -CONHOCO-. The printing plate master shows improved stability.

ACCESSION NUMBER: 2004:37360 CAPLUS
DOCUMENT NUMBER: 140:84686
TITLE: Positive-working offset printing plate master suitable for IR laser digital direct platemaking
INVENTOR(S): Endo, Akihiro
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 27 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004012978	A2	20040115	JP 2002-168556	20020610
PRIORITY APPLN. INFO.:			JP 2002-168556	20020610

IT **640285-80-9**
RL: MOA (Modifier or additive use); USES (Uses)
(organic acid precursor; pos.-working offset printing plate master containing organic acid precursor suitable for IR laser digital direct platemaking)
RN 640285-80-9 CAPLUS
CN Benzaldehyde, 2,4-dimethoxy-, O,O'-(1,2-phenylenedicarbonyl)dioxime (9CI) (CA INDEX NAME)





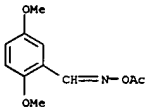
L27 ANSWER 2 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN
AB The title composition contains alkali soluble composition materials, oxime ester as a polymerization initiator, and photopolymg. materials, wherein the oxime ester has structure Ar1-C=NOR1(H) or M1-[-C=NOR1(H)]x (R1 = cycloalkanoyl, benzoyl, alkenoyl; Ar1 = aryl, aroyl; M1 = 2, 3). The composition, which contain the oxime ester, provides the photoresist of the improved resolution and shows the good storageability.

ACCESSION NUMBER: 2001:752027 CAPLUS
DOCUMENT NUMBER: 135:264637
TITLE: Light-sensitive photoresist composition containing oxime esters as polymerization initiator in fabrication of optical filters in optical imaging devices
INVENTOR(S): Oka, Hidetaka; Kunimoto, Kazuhiko; Kura, Hisatoshi; Ohwa, Masaki; Tanabe, Junichi
PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.
SOURCE: Fr. Demande, 110 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

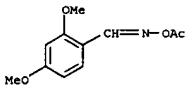
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
FR 2802655	A1	20010622	FR 2000-16309		20001214
FR 2802655	B1	20030815			
SG 97168	A1	20030718	SG 2000-6382		20001103
NL 1016814	A1	20010618	NL 2000-1016814		20001206
NL 1016814	C2	20020129			
GB 2357293	A1	20010620	GB 2000-29801		20001207
GB 2357293	B2	20020807			
SE 2000004565	A	20010725	SE 2000-4565		20001211
SE 522645	C2	20040224			
JP 2001235858	A2	20010831	JP 2000-376036		20001211
US 2002020832	A1	20020221	US 2000-734635		20001212
IT 1319687	B1	20031023	IT 2000-MI2675		20001212
CA 2328342	AA	20010615	CA 2000-2328342		20001213
FI 2000002731	A	20010616	FI 2000-2731		20001213
DE 10061948	A1	20010621	DE 2000-10061948		20001213
BR 2000005866	A	20020521	BR 2000-5866		20001213
CN 1305124	A	20010725	CN 2000-135063		20001214
BE 1013705	A3	20020604	BE 2000-786		20001214
AT 200002080	A5	20020615	AT 2000-2080		20001214
AT 410146	B	20030225			
ES 2189609	A1	20030701	ES 2000-2990		20001214
ES 2189609	B1	20040401			
AU 773749	B2	20040603	AU 2000-72268		20001214
PRIORITY APPLN. INFO.:			EP 1999-811161	A	19991215
			EP 2000-810630	A	20000717

IT **122913-67-1P 362523-27-1P**
RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

L27 ANSWER 2 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
(oxime in light-sensitive color filter compn.)
RN 122913-67-1 CAPLUS
CN Benzaldehyde, 2,5-dimethoxy-, O-acetyloxime (9CI) (CA INDEX NAME)



RN 362523-27-1 CAPLUS
CN Benzaldehyde, 2,4-dimethoxy-, O-acetyloxime (9CI) (CA INDEX NAME)



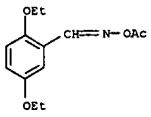
L27 ANSWER 3 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN
AB The invention relates to a photopolymn. initiator of oxime ester for a photoresist composition, wherein the oxime is derivative of Ar1-C=N-OR1(H) (R1 = cycloalkanoyl, benzoyl, alkenoyl; Ar1 = aryl, aroyl). The photopolymn. initiator provides the alkali-developable light-sensitive photoresist composition, which shows the improved storageability, of the high resolution and the good storageability.

ACCESSION NUMBER: 2001:752026 CAPLUS
DOCUMENT NUMBER: 135:280493
TITLE: Photopolymerization initiator of oxime ester for light-sensitive photoresist composition
INVENTOR(S): Kunimoto, Kazuhiko; Oka, Hidetaka; Ohwa, Masaki; Tanabe, Junichi; Kura, Hisatoshi; Birbaum, Jean Luc
PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.
SOURCE: Fr. Demande, 171 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

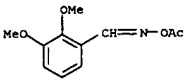
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
FR 2802528	A1	20010622	FR 2000-16306		20001214
TW 499411	B	20020821	TW 2000-89123924		20001110
NL 1016815	A1	20010618	NL 2000-1016815		20001206
NL 1016815	C2	20020514			
GB 2358017	A1	20010711	GB 2000-29793		20001207
GB 2358017	B2	20020313			
SE 2000004564	A	20020612	SE 2000-4564		20001211
SE 522774	C2	20040302			
US 2001012596	A1	20010809	US 2000-734625		20001212
JP 2001233842	A2	20010828	JP 2000-377671		20001212
IT 1319688	B1	20031023	IT 2000-MI2676		20001212
CA 2328376	AA	20010615	CA 2000-2328376		20001213
FI 2000002730	A	20010616	FI 2000-2730		20001213
DE 10061947	A1	20010621	DE 2000-10061947		20001213
ES 2177438	A1	20021201	ES 2000-2977		20001213
ES 2177438	B1	20041016			
DK 200001878	A5	20010616	DK 2000-1878		20001214
BE 1013872	A5	20021105	BE 2000-789		20001214
CN 1299812	A	20010620	CN 2000-135980		20001215
BR 2000006379	A	20010724	BR 2000-6379		20001215
PRIORITY APPLN. INFO.:			EP 1999-811160	A	19991215
			EP 2000-810629	A	20000717

IT **362624-54-2P 362624-55-3P 362624-56-4P 362624-57-5P 362624-58-6P 362624-72-4P 362624-82-6P 362624-83-7P 362624-99-5P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(light-sensitive color filter composition containing oxime esters used in optical imaging devices)
RN 362624-54-2 CAPLUS
CN Benzaldehyde, 2,5-diethoxy-, O-acetyloxime (9CI) (CA INDEX NAME)

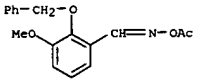
L27 ANSWER 3 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



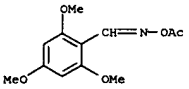
RN 362624-55-3 CAPLUS
CN Benzaldehyde, 2,3-dimethoxy-, O-acetyloxime (9CI) (CA INDEX NAME)



RN 362624-56-4 CAPLUS
CN Benzaldehyde, 3-methoxy-2-(phenylmethoxy)-, O-acetyloxime (9CI) (CA INDEX
NAME)

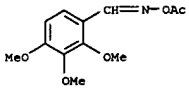


RN 362624-57-5 CAPLUS
CN Benzaldehyde, 2,4,6-trimethoxy-, O-acetyloxime (9CI) (CA INDEX NAME)

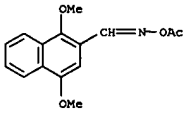


RN 362624-58-6 CAPLUS
CN Benzaldehyde, 2,3,4-trimethoxy-, O-acetyloxime (9CI) (CA INDEX NAME)

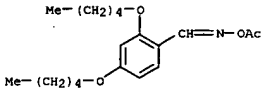
L27 ANSWER 3 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



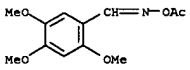
RN 362624-72-4 CAPLUS
CN 2-Naphthalenecarboxaldehyde, 1,4-dimethoxy-, O-acetyloxime (9CI) (CA INDEX NAME)



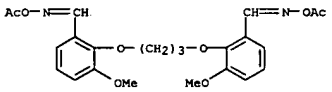
RN 362624-82-6 CAPLUS
CN Benzaldehyde, 2,4-bis(pentyloxy)-, O-acetyloxime (9CI) (CA INDEX NAME)



RN 362624-83-7 CAPLUS
CN Benzaldehyde, 2,4,5-trimethoxy-, O-acetyloxime (9CI) (CA INDEX NAME)



RN 362624-99-5 CAPLUS
CN Benzaldehyde, 2,2'-[1,3-propanediylbis(oxy)]bis[3-methoxy-, bis(O-acetyloxime) (9CI) (CA INDEX NAME)



L27 ANSWER 3 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

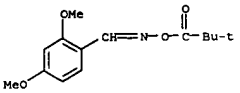
L27 ANSWER 4 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN

AB Photolyses of aldoxime esters, containing a considerable range of alkyl groups, lead to cleavage of their N-O bonds and formation of aryliminyl and alkyl radicals. The process was found to be favored by 4-methoxyacetophenone as a photosensitizer and by methoxy substituents in the aryl rings. 4-Nitro- and pentafluoro-substitutions of the aryl rings were, on the other hand, deleterious. The intermediate iminyl radicals, together with primary, secondary and tertiary alkyl radicals were characterized by 9 GHz EPR spectroscopy. Cyclopropyl, CF3, and CCl3 radicals were probably also formed, but were too reactive for direct EPR spectroscopic detection. Photosensitized reaction of benzophenone oxime O-nonanoyl ester produced the diphenylmethaniminoxyl, as well as the expected n-octyl and iminyl radicals. This indicated that O-C bond scission accompanied O-N scission for this ketoxime ester. At higher temps. the C-centered radicals added to the starting oxime esters to produce alkoxyaminyl radicals that were also spectroscopically detected in some cases. No evidence for abstraction of the iminyl hydrogen by tert-butoxyl radicals was obtained. Instead, the t-BuO• radicals added to the C:N double bonds of the oxime esters. Similarly, chlorine abstraction from alkylbenzohydroximoyl chlorides by trimethyltin radicals did not take place. Preparative scale expts. with oxime esters containing suitably unsatd. alkyl groups showed that good yields of cyclised products could be obtained in the presence of the photosensitizer. This process constitutes a general method by which carboxylic acids or acid chlorides can be converted into alkyl radicals and hence to cyclized derivs.

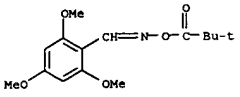
ACCESSION NUMBER: 2000:832599 CAPLUS
DOCUMENT NUMBER: 134:178233
TITLE: Exploitation of aldoxime esters as radical precursors in preparative and EPR spectroscopic roles
AUTHOR(S): McCarroll, Andrew J.; Walton, John C.
CORPORATE SOURCE: University of St. Andrews, School of Chemistry, St Andrews, Fife, KY16 9ST, UK
SOURCE: Perkin 2 (2000), (12), 2399-2409
CODEN: PRKTFO; ISSN: 1470-1820
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:178233

IT **265122-24-5P 265122-25-6P 265122-28-9P 265122-29-0P 265122-30-3P 265122-31-4P 265122-33-6P 265122-34-7P 265122-35-8P 265122-36-9P 326853-06-9P 326853-07-0P 326853-08-1P 326853-09-2P 326853-10-5P 326853-11-6P**
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(photolysis; preparative and ESR studies of the photolysis of aldoxime esters as radical precursors)

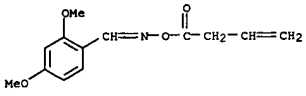
RN 265122-24-5 CAPLUS
CN Benzaldehyde, 2,4-dimethoxy-, O-(2,2-dimethyl-1-oxopropyl)oxime (9CI) (CA INDEX NAME)



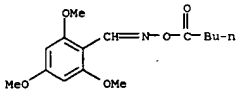
RN 265122-25-6 CAPLUS
CN Benzaldehyde, 2,4,6-trimethoxy-, O-(2,2-dimethyl-1-oxopropyl)oxime (9CI) (CA INDEX NAME)



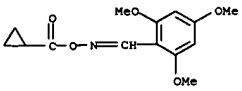
RN 265122-28-9 CAPLUS
CN Benzaldehyde, 2,4-dimethoxy-, O-(1-oxo-3-butenyl)oxime (9CI) (CA INDEX NAME)



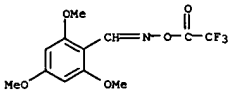
RN 265122-29-0 CAPLUS
CN Benzaldehyde, 2,4,6-trimethoxy-, O-(1-oxopentyl)oxime (9CI) (CA INDEX NAME)



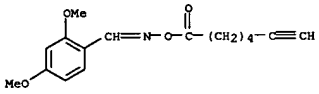
RN 265122-30-3 CAPLUS
CN Benzaldehyde, 2,4,6-trimethoxy-, O-(cyclopropylcarbonyl)oxime (9CI) (CA INDEX NAME)



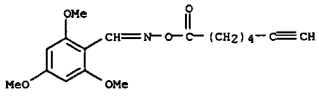
RN 265122-31-4 CAPLUS
CN Benzaldehyde, 2,4,6-trimethoxy-, O-(trifluoroacetyl)oxime (9CI) (CA INDEX NAME)



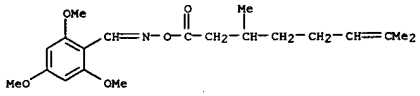
RN 265122-33-6 CAPLUS
CN Benzaldehyde, 2,4-dimethoxy-, O-(1-oxo-6-heptynyl)oxime (9CI) (CA INDEX NAME)



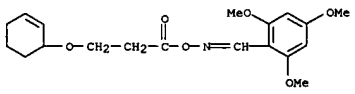
RN 265122-34-7 CAPLUS
CN Benzaldehyde, 2,4,6-trimethoxy-, O-(1-oxo-6-heptynyl)oxime (9CI) (CA INDEX NAME)



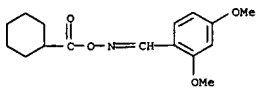
RN 265122-35-8 CAPLUS
CN Benzaldehyde, 2,4,6-trimethoxy-, O-(3,7-dimethyl-1-oxo-6-octenyl)oxime (9CI) (CA INDEX NAME)



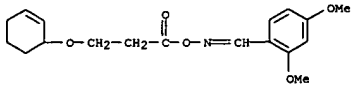
RN 265122-36-9 CAPLUS
CN Benzaldehyde, 2,4,6-trimethoxy-, O-[3-(2-cyclohexen-1-yloxy)-1-oxopropyl]oxime (9CI) (CA INDEX NAME)



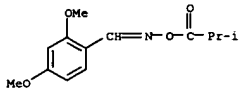
RN 326853-06-9 CAPLUS
CN Benzaldehyde, 2,4-dimethoxy-, O-(cyclohexylcarbonyl)oxime (9CI) (CA INDEX NAME)



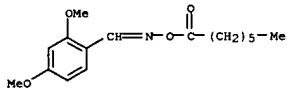
RN 326853-07-0 CAPLUS
CN Benzaldehyde, 2,4-dimethoxy-, O-[3-(2-cyclohexen-1-yloxy)-1-oxopropyl]oxime (9CI) (CA INDEX NAME)



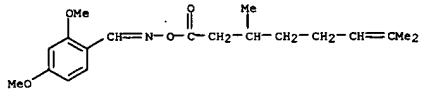
RN 326853-08-1 CAPLUS
CN Benzaldehyde, 2,4-dimethoxy-, O-(2-methyl-1-oxopropyl)oxime (9CI) (CA INDEX NAME)



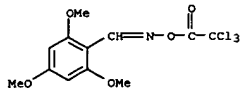
RN 326853-09-2 CAPLUS
CN Benzaldehyde, 2,4-dimethoxy-, O-(1-oxoheptyl)oxime (9CI) (CA INDEX NAME)



RN 326853-10-5 CAPLUS
CN Benzaldehyde, 2,4-dimethoxy-, O-(3,7-dimethyl-1-oxo-6-octenyl)oxime (9CI) (CA INDEX NAME)



RN 326853-11-6 CAPLUS
CN Benzaldehyde, 2,4,6-trimethoxy-, O-(trichloroacetyl)oxime (9CI) (CA INDEX NAME)



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

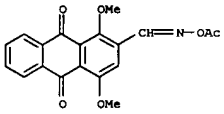
L27 ANSWER 5 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN

AB 2-(1-Hydroxyiminoalkyl)-1,4-dimethoxy-9,10-anthraquinones were demethylated to produce 2-(1-hydroxyiminoalkyl)-1,4-dihydroxy-9,10-anthraquinones (1,4-dihydroxy-9,10-anthraquinone, DHAQ), and oxime hydroxyl groups were in turn acylated to give the corresponding 2-(1-acyloxyiminoalkyl)-DHAQ derivs. The anti-proliferative activity of 2-(1-hydroxyiminoalkyl)-DHAQ derivs. was found to be dependent on the size of the alkyl chain. Thus, DHAQ analogs with alkyl chains longer than heptyl had negligible anti-proliferative activity, while those compds. possessing shorter chains demonstrated moderate anti-proliferative activity (ED50, 2.73-19.21 μM). However, the antitumor activity as expressed by T/C values did not correlate with the anti-proliferative activity; 2-(1-hydroxyiminononyl)-DHAQ with an ED50 value of >20 μM exhibited potent antitumor activity (T/C, 166%). Only four of the 2-(1-hydroxyiminoalkyl)-DHAQ analogs showed good antitumor activity (T/C, >150%): 2-(1-hydroxyiminobutyl)-DHAQ (T/C, 163%), 2-(1-hydroxyiminopentyl)-DHAQ (T/C, 180%) and 2-(1-hydroxyiminononyl)-DHAQ (T/C, 166%). Acylation of the hydroxyl group of these oximes enhanced the anti-proliferative activity and antitumor effects: 2-(1-propanoyloxyiminopropyl)-DHAQ (ED50, 4.41 μM; T/C, 221%) vs. 2-(1-hydroxyiminopropyl)-DHAQ (ED50, 14.64 μM; T/C, 100%) and 2-(1-propanoyloxyiminobutyl)-DHAQ (ED50, 2.65 μM; T/C, 202%) vs. 2-(1-hydroxyiminobutyl)-DHAQ (ED50, 16.43 μM; T/C, 163%).

ACCESSION NUMBER: 2000:459209 CAPLUS
DOCUMENT NUMBER: 133:222418
TITLE: Synthesis and evaluation of the antitumor activity of 2-substituted 1,4-dihydroxy-9,10-anthraquinones
AUTHOR(S): Tam, Mai-Ngoc; Nam, Nguyen-Hai; Jin, Guang-Zu; Song, Gyu-Yong; Ahn, Byung-Zun
CORPORATE SOURCE: Institute of Building Materials, Hanoi, Vietnam
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (2000), 333(6), 189-194
CODEN: ARPMAS; ISSN: 0365-6233
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **291749-15-0P 291749-25-2P 291749-34-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and antitumor activity of 2-substituted 1,4-dihydroxyanthraquinones)

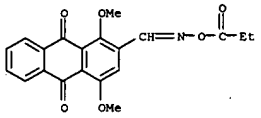
RN 291749-15-0 CAPLUS
CN 2-Anthracenecarboxaldehyde, 9,10-dihydro-1,4-dimethoxy-9,10-dioxo-, 2-(O-acetyloxime) (9CI) (CA INDEX NAME)



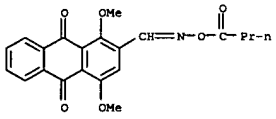
RN 291749-25-2 CAPLUS
CN 2-Anthracenecarboxaldehyde, 9,10-dihydro-1,4-dimethoxy-9,10-dioxo-,

L27 ANSWER 5 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

2-[O-(1-oxopropyl)oxime] (9CI) (CA INDEX NAME)



RN 291749-34-3 CAPLUS
CN 2-Anthracenecarboxaldehyde, 9,10-dihydro-1,4-dimethoxy-9,10-dioxo-, 2-[O-(1-oxobutyl)oxime] (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

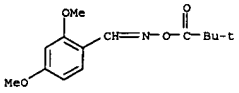
L27 ANSWER 6 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN

AB Arylmethaniminyl and alkyl radicals were generated from di- and tri-methoxyphenyl aldoxime esters, by photolysis in the presence of 4-methoxyacetophenone, and were detected by EPR spectroscopy: good yields of cyclized products were isolated from suitably unsatd. alkyl substituents.

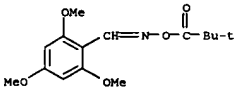
ACCESSION NUMBER: 2000:133509 CAPLUS
DOCUMENT NUMBER: 132:308008
TITLE: Enhanced radical delivery from aldoxime esters for EPR and ring closure applications
AUTHOR(S): McCarroll, Andrew J.; Walton, John C.
CORPORATE SOURCE: Sch. Chem., University of St. Andrews, St. Andrews, Fife, KY16 9ST, UK
SOURCE: Chemical Communications (Cambridge) (2000), (5), 351-352
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:308008

IT **265122-24-5 265122-25-6 265122-28-9 265122-29-0 265122-30-3 265122-31-4 265122-33-6 265122-34-7 265122-35-8 265122-36-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(photolysis; ESR study of arylmethaniminyl and alkyl radical formation in sensitized photolysis of aryl aldoxime esters and preparative decarboxylative cyclization of unsatd. carboxylic acids via aldoxime ester photolysis)

RN 265122-24-5 CAPLUS
CN Benzaldehyde, 2,4-dimethoxy-, O-(2,2-dimethyl-1-oxopropyl)oxime (9CI) (CA INDEX NAME)

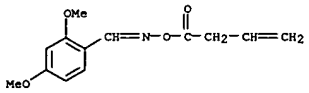


RN 265122-25-6 CAPLUS
CN Benzaldehyde, 2,4,6-trimethoxy-, O-(2,2-dimethyl-1-oxopropyl)oxime (9CI) (CA INDEX NAME)

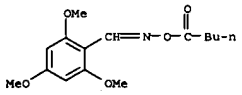


RN 265122-28-9 CAPLUS
CN Benzaldehyde, 2,4-dimethoxy-, O-(1-oxo-3-butenyl)oxime (9CI) (CA INDEX NAME)

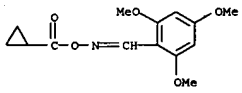
L27 ANSWER 6 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



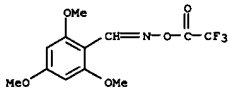
RN 265122-29-0 CAPLUS
CN Benzaldehyde, 2,4,6-trimethoxy-, O-(1-oxopentyl)oxime (9CI) (CA INDEX NAME)



RN 265122-30-3 CAPLUS
CN Benzaldehyde, 2,4,6-trimethoxy-, O-(cyclopropylcarbonyl)oxime (9CI) (CA INDEX NAME)

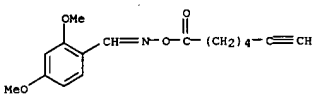


RN 265122-31-4 CAPLUS
CN Benzaldehyde, 2,4,6-trimethoxy-, O-(trifluoroacetyl)oxime (9CI) (CA INDEX NAME)

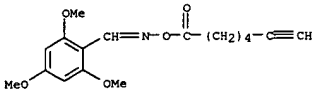


RN 265122-33-6 CAPLUS
CN Benzaldehyde, 2,4-dimethoxy-, O-(1-oxo-6-heptynyl)oxime (9CI) (CA INDEX NAME)

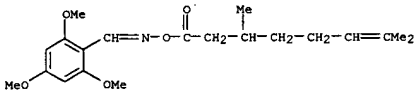
L27 ANSWER 6 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



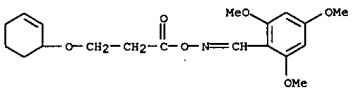
RN 265122-34-7 CAPLUS
CN Benzaldehyde, 2,4,6-trimethoxy-, O-(1-oxo-6-heptynyl)oxime (9CI) (CA INDEX NAME)



RN 265122-35-8 CAPLUS
CN Benzaldehyde, 2,4,6-trimethoxy-, O-(3,7-dimethyl-1-oxo-6-octenyl)oxime (9CI) (CA INDEX NAME)

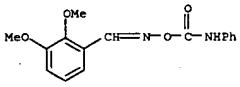


RN 265122-36-9 CAPLUS
CN Benzaldehyde, 2,4,6-trimethoxy-, O-[3-(2-cyclohexen-1-yloxy)-1-oxopropyl]oxime (9CI) (CA INDEX NAME)



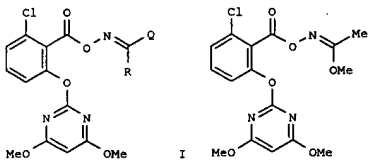
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L27 ANSWER 7 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN
AB O-arylcarbamoylated hydroxylamine tosylate reacts with aldehydes at room temperature to give the corresponding O-carbamoylated oximes. The reaction of carbamoylated hydroxylamine with aromatic aldehydes in THF or in toluene at reflux affords the corresponding nitriles and anilinium tosylate in high yield. Attempts to cyclize the O-carbamoylated oximes in the presence of AcCl lead again to the formation of nitriles.
ACCESSION NUMBER: 1999:631975 CAPLUS
DOCUMENT NUMBER: 132:3107
TITLE: Direct conversion of aldehydes to nitriles via O-phenylcarbamoylated aldoximes
AUTHOR(S): Coskun, Necdet; Arikan, Nevin
CORPORATE SOURCE: Department of Chemistry, Uludag University, Bursa, 16059, Turk.
SOURCE: Tetrahedron (1999), 55(40), 11943-11948
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:3107
IT **250722-17-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(direct conversion of aldehydes to nitriles via O-phenylcarbamoylated aldoximes)
RN 250722-17-9 CAPLUS
CN Benzaldehyde, 2,3-dimethoxy-, O-[(phenylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L27 ANSWER 8 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN
GI



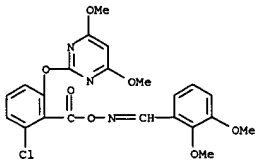
AB New 6-chloro-2-[(4,6-dimethoxy-2-pyrimidinyl)oxy]benzoates [[2-[[(alkyleneamino)oxy]carbonyl]-1-chloro-3-phenoxy]pyrimidines] I (R = H, halo, cyano, etc.; Q = alkyl, alkenyl, cycloalkyl, etc.) were disclosed. I were claimed as herbicides. An example compound 2-[1-chloro-[[[(1-methoxyethylidene)amino]oxy]carbonyl]phenoxy]-4,6-dimethoxypyrimidine (II) was prepared
ACCESSION NUMBER: 1994:605344 CAPLUS
DOCUMENT NUMBER: 121:205344
TITLE: Novel 6-chloro-2-(4,6-dimethoxypyrimidin-2-yl) oxybenzoic acid ester derivatives, processes for their production and their application as herbicides.
INVENTOR(S): Hur, Chang Uk; Cho, Jin Ho; Lee, Ho Seong; Yoo, Sang Ku; Hong, Su Myeong; Kim, Hong Woo; Rim, Jae Suk; Bae, Yeong Tae; Chae, Sand Heon; et al.
PATENT ASSIGNEE(S): Lucky Ltd., S. Korea
SOURCE: Eur. Pat. Appl., 82 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 608862	A1	19940803	EP 1994-101132	19940126
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
KR 9603323	B1	19960308	KR 1993-1017	19930127
KR 9612180	B1	19960916	KR 1993-10097	19930604
KR 9612179	B1	19960916	KR 1993-10098	19930604
KR 9612181	B1	19960916	KR 1993-10099	19930604
KR 9612194	B1	19960916	KR 1993-10100	19930604
KR 9612195	B1	19960916	KR 1993-10101	19930604
CN 1101345	A	19950412	CN 1994-102665	19940126
US 5494888	A	19960227	US 1994-186589	19940126
BR 9400365	A	19940816	BR 1994-365	19940127
JP 07149735	A2	19950613	JP 1994-7824	19940127
JP 2543665	B2	19961016		
IN 182571	A	19990508	IN 1994-DE86	19940128
IN 183197	A	19991002	IN 1994-DE1445	19941111

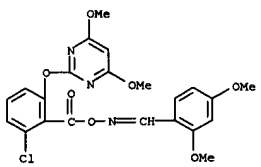
L27 ANSWER 8 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PRIORITY APPLN. INFO.:	KR 1993-1017	A 19930127
	KR 1993-10097	A 19930604
	KR 1993-10098	A 19930604
	KR 1993-10099	A 19930604
	KR 1993-10100	A 19930604
	KR 1993-10101	A 19930604
	EP 1994-101132	A 19940126

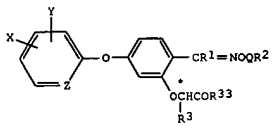
OTHER SOURCE(S): MARPAT 121:205344
IT **157990-33-5P 157990-35-7P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide)
RN 157990-33-5 CAPLUS
CN Benzaldehyde, 2,3-dimethoxy-, O-[2-chloro-6-[(4,6-dimethoxy-2-pyrimidinyl)oxy]benzoyl]oxime (9CI) (CA INDEX NAME)



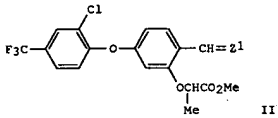
RN 157990-35-7 CAPLUS
CN Benzaldehyde, 2,4-dimethoxy-, O-[2-chloro-6-[(4,6-dimethoxy-2-pyrimidinyl)oxy]benzoyl]oxime (9CI) (CA INDEX NAME)



L27 ANSWER 9 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN
GI



I



II

AB The title compds. [I; X, Y H, halo, CF3, C1-5 alkyl; Z = CH, N; R1 = H, HO, C1-5 alkyl or alkoxy; R2 = (un)substituted C1-10 (un)saturated aliphatic hydrocarbon group, alkoxy, PhO, C6-20 aromatic hydrocarbon group, NH2, C3-20 aromatic heterocyclyl containing at least one N atom.; R3 = C1-5 alkyl, Ph; R33 = HO, C1-5 (halo)alkyl, (halo)phenyl, carboxy- or alkoxycarbonyl-substituted C1-5 alkoxy, C1-5 alkenyloxy, (un)substituted NH2, NHP(O)(OR10)OR11; R10, R11 = H, C1-5 alkyl, Ph; Q = direct bond, CO, C(S), SO2; when Q = direct bond, R2 = (un)substituted alkoxy, PhO, or C6-20 aromatic hydrocarbon group] are prepared Thus, tosylation of Me (S)-(-)-lactate by tosyl chloride in benzene containing Et3N and etherification of the resulting Me O-(p-toluenesulfonyl)-(S)-(-)-lactate with 2-hydroxy-4-(2-chloro-4-trifluoromethylphenoxy)benzaldehyde in refluxing MeCN containing K2CO3 gave a benzaldehyde derivative (II; Z1 = O) which was condensed with O-(4-nitrophenyl)hydroxylamine in THF containing one drop of concentrated HCl to give II (Z1 = NC6H4NO2-p) (III). III at 0.125 kg/ha postemergence completely controlled 9 weeds, e.g., Digitaria sp., Setaria viridis, and Abutilon avicennae. A mixture III and N-(phosphonomethyl)glycine isopropylamine salt showed synergistic herbicidal activity against true glass and broad leaf weeds.

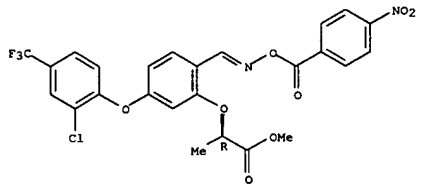
ACCESSION NUMBER: 1994:270126 CAPLUS
DOCUMENT NUMBER: 120:270126
TITLE: Preparation of pyridyloxy- and phenoxybenzaldehyde oxime derivatives as herbicides
INVENTOR(S): Azuma, Shizuo; Hiramatsu, Toshuki; Ichikawa, Yataro
PATENT ASSIGNEE(S): Teijin Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 45 pp.

L27 ANSWER 9 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05320117	A2	19931203	JP 1991-23791	19910125
PRIORITY APPLN. INFO.:			JP 1990-13478	A1 19900125

OTHER SOURCE(S): MARPAT 120:270126
IT **154317-18-7P 154317-33-6P 154317-34-7P 154317-35-8P 154317-37-0P 154317-38-1P 154317-39-2P 154317-40-5P 154317-41-6P 154317-42-7P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as herbicide)
RN 154317-18-7 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[(4-nitrobenzoyl)oxy]imino]methyl]phenoxy]-, methyl ester, (R)- (9CI) (CA INDEX NAME)

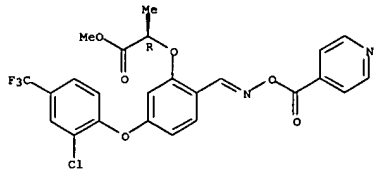
Absolute stereochemistry.
Double bond geometry unknown.



RN 154317-33-6 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[(4-pyridinylcarbonyl)oxy]imino]methyl]phenoxy]-, methyl ester, (R)- (9CI) (CA INDEX NAME)

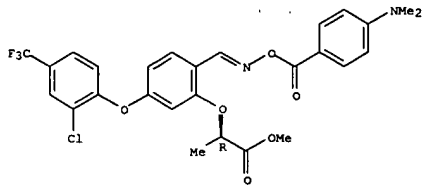
Absolute stereochemistry.
Double bond geometry unknown.

L27 ANSWER 9 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



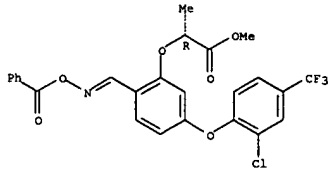
RN 154317-34-7 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[[4-(dimethylamino)benzoyl]oxy]imino]methyl]phenoxy]-, methyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



RN 154317-35-8 CAPLUS
CN Propanoic acid, 2-[2-[[(benzoyloxy)imino]methyl]-5-[2-chloro-4-(trifluoromethyl)phenoxy]phenoxy]-, methyl ester, (R)- (9CI) (CA INDEX NAME)

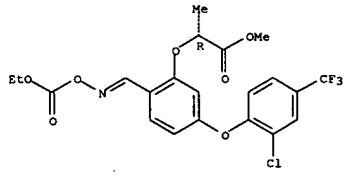
Absolute stereochemistry.
Double bond geometry unknown.



L27 ANSWER 9 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

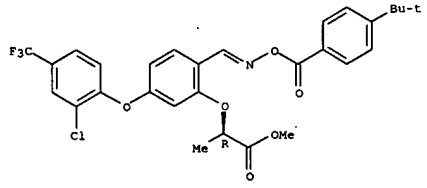
RN 154317-37-0 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[(ethoxycarbonyl)oxy]imino]methyl]phenoxy]-, methyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



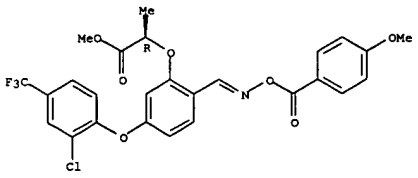
RN 154317-38-1 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[[4-(1,1-dimethylethyl)benzoyl]oxy]imino]methyl]phenoxy]-, methyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



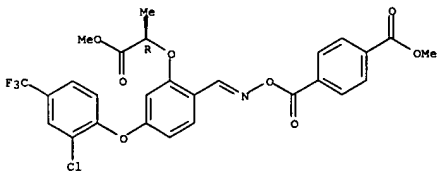
RN 154317-39-2 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[(4-methoxybenzoyl)oxy]imino]methyl]phenoxy]-, methyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



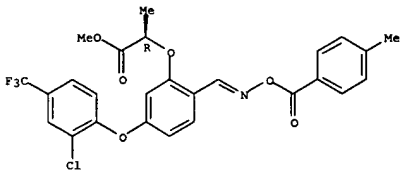
RN 154317-40-5 CAPLUS
CN Benzoic acid, 4-[[[[[4-[2-chloro-4-(trifluoromethyl)phenoxy]-2-(2-methoxy-1-methyl-2-oxoethoxy)phenyl]methylene]amino]oxy]carbonyl]-, methyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



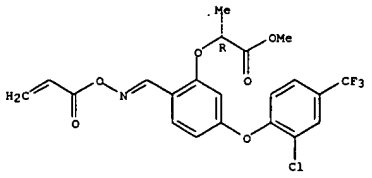
RN 154317-41-6 CAPLUS
CN Propanoic acid, 2-(5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[(4-methylbenzoyl)oxy]imino]methyl]phenoxy]-, methyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

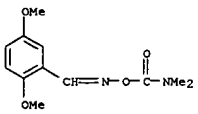


RN 154317-42-7 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[(1-oxo-2-propenyl)oxy]imino]methyl]phenoxy]-, methyl ester, (R)- (9CI) (CA INDEX NAME)

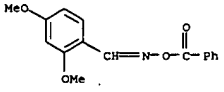
Absolute stereochemistry.
Double bond geometry unknown.



AB Thermal decomposition of syn-RCH:NOCONMe2 [I: R = 2-pyridyl, 4-C6H4NO2, Ph, 4-C6H4NMe2, 2,4- or 2,5-C6H3(OMe)2, 2-methyl- or 2-methoxy-4-dimethylaminophenyl, 2-methoxy-1-naphthyl] and syn-RCH:NOBz [II: R = Ph, 4-C6H4OMe, 2,4-C6H3(OMe)2, 2- or 4-methoxy-1-naphthyl, 1,5-C10H6SO2NEt2, 2-benzyloxy-1-naphthyl] at 80-130° was kinetically studied. The decomposition was 1st-order for both I and II, and electron donating groups and substituents at the ortho position increased the reaction rates. Activation entropy values for I and II were very different and, hence, different decomposition mechanisms were proposed: β-elimination with syn/anti isomerization for I and concerted elimination via a cyclic 6-membered ring transition for II.
ACCESSION NUMBER: 1992:469340 CAPLUS
DOCUMENT NUMBER: 117:69340
TITLE: Reaction control of thermal decomposition of aromatic aldoxime derivatives as heat decomposing precursor compounds
AUTHOR(S): Kawata, Ken; Kitaguchi, Hiroshi; Sato, Kozo; Yabuki, Yoshiharu
CORPORATE SOURCE: Ashigara Res. Lab., Fuji Photo Film Co., Ltd., Kanagawa, 250-01, Japan
SOURCE: Senryo to Yakuhin (1992), 37(2), 33-40
CODEN: SETYAL; ISSN: 0370-9671
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
IT **93369-34-7 99806-97-0 142554-03-8**
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(thermal decomposition of, kinetics of, substituent effect and mechanism in relation to)
RN 93369-34-7 CAPLUS
CN Benzaldehyde, 2,5-dimethoxy-, O-[(dimethylamino)carbonyl]oxime (9CI) (CA INDEX NAME)

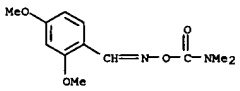


RN 99806-97-0 CAPLUS
CN Benzaldehyde, 2,4-dimethoxy-, O-benzoyloxime (9CI) (CA INDEX NAME)



RN 142554-03-8 CAPLUS

CN Benzaldehyde, 2,4-dimethoxy-, O-[(dimethylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



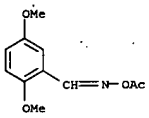
L27 ANSWER 11 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN

AB RCH2NR1CH2CONR2(OH) (I; R = insol. polymer residue; R1, R2 = alkyl), useful for selective deacylation in an organic solvent under neutral conditions, are prepared by reaction of CH2Cl group-containing polymers with N-hydroxy-N-alkyl(alkyl)aminoacetamides. Thus, 40 g MeNHOH.HCl was treated with 25 g MeNHCH2CO2Me in H2O/MeOH containing NaOH to give 26 g MeNHCH2CONMe(OH), which was treated with 5 g Bio-Beads S-X1 (p-chloromethylstyrene-divinylbenzene copolymer) to give 4.7 g I (R = polymer residue; R1 = R2 = Me), which selectively deacetylated p-acetylaminophenyl acetate in EtOH at 45° to give p-acetylaminophenol in 70% yield.

ACCESSION NUMBER: 1991:516809 CAPLUS
DOCUMENT NUMBER: 115:116809
TITLE: Polymer-supported deacylation agents.
INVENTOR(S): Ono, Mitsunori
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03072434	A2	19910327	JP 1989-186248	19890719
US 5116994	A	19920526	US 1990-509826	19900417
PRIORITY APPLN. INFO.:			JP 1989-99225 A1	19890419
			JP 1989-186248 A	19890719

IT **122913-67-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(deacetylation of, with hydroxamic acid derivs. fixed on polymer beads)
RN 122913-67-1 CAPLUS
CN Benzaldehyde, 2,5-dimethoxy-, O-acetyloxime (9CI) (CA INDEX NAME)



L27 ANSWER 12 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN

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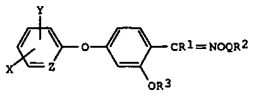

I

AB Oxime derivs. I (X, Y, Z, R1, R2, R3 and Q are defined) showed excellent herbicidal effect against broad- and narrow-leaved weeds and had quick acting herbicidal activity. Preparation of these compds. by 2 different schemes is described. Thus, 3-(2-chloro-4-trifluoromethylphenoxy)phenol in CH2Cl2 was treated with TiCl4 then by dichloromethyl Me ether, and the product (2-hydroxy-4-(2-chloro-4-trifluoromethylphenoxybenzaldehyde) was refluxed with EtI, K2CO3 and MeEt ketone to give 2-ethoxy-4-(2-chloro-4-trifluoromethylphenoxy)benzaldehyde which was treated with NH2OH.HCl to give 2-ethoxy-4-(2-chloro-4-trifluoromethylphenyoxy)benzaldehyde oxime (I, R1 = R2 = H; R3 = Et; X = CF3; Y = Cl; Z = CH:) (II). Formulations of II at 0.5 kg/h were 100% effective against Abutilon theophrasti. I (R1 = R2 = H; R3 = CH(Me)CO2Me; X = CF3; Y = Cl; Z = -CH:) was 100% effective against Chenopodium album centrorubrum, Aranthus mangostanus, Astragalus sinicus, A. theophrasti, Solanum nigrum, and Xanthium strumarium.

ACCESSION NUMBER: 1990:436398 CAPLUS
DOCUMENT NUMBER: 113:36398
TITLE: Oxime derivatives and herbicides containing the same as an active ingredient
INVENTOR(S): Azuma, Shizuo; Nakagawa, Koji; Hiramatsu, Toshiyuki; Ichikawa, Yataro
PATENT ASSIGNEE(S): Teijin Ltd., Japan
SOURCE: PCT Int. Appl., 148 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9001874	A1	19900308	WO 1989-JP864	19890823
W: AU, BG, DK, FI, HU, JP, KR, NO, RO, SU, US				
RW: BE, CH, DE, FR, GB, IT, NL, SE				
WO 9002113	A1	19900308	WO 1988-JP837	19880824
W: AU, JP, KR, US				
RW: CH, DE, FR, GB				
AU 8940752	A1	19900323	AU 1989-40752	19890823
AU 619038	B2	19920116		
EP 433451	A1	19910626	EP 1989-909629	19890823
R: BE, CH, DE, FR, GB, IT, LI, NL, SE				
JP 04500074	T2	19920109	JP 1989-509021	19890823
ZA 9001158	A	19901128	ZA 1990-1158	19900215
PRIORITY APPLN. INFO.:			WO 1988-JP837 A	19880824
			JP 1989-30002 A	19890210

L27 ANSWER 12 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

JP 1989-130002	A	19890210
WO 1989-JP864	A	19890823

OTHER SOURCE(S): MARPAT 113:36398

IT **128079-35-6P 128079-36-7P 128079-37-8P**
128079-38-9P 128079-39-0P 128079-40-3P
128079-42-5P 128079-43-6P 128079-44-7P
128079-45-8P 128079-46-9P 128079-47-0P
128079-48-1P 128079-49-2P 128079-50-5P
128079-51-6P 128079-52-7P 128079-53-8P
128079-54-9P 128079-55-0P 128079-57-2P
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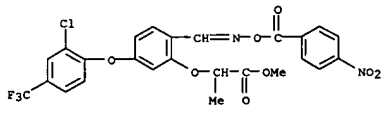
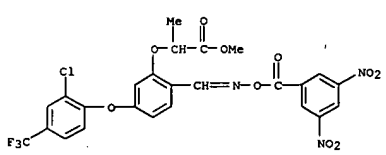
128079-61-8P 128079-62-9P 128079-63-0P
128079-64-1P 128079-65-2P 128079-66-3P
128079-67-4P 128079-68-5P 128079-69-6P
128079-70-9P 128079-71-0P 128079-73-2P
128079-74-3P 128079-75-4P 128096-69-5P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and herbicidal activity of)

RN 128079-35-6 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[(4-nitrobenzoyl)oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)

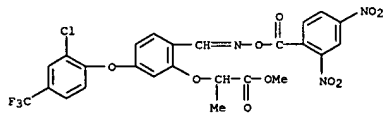


RN 128079-36-7 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[(3,5-dinitrobenzoyl)oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)

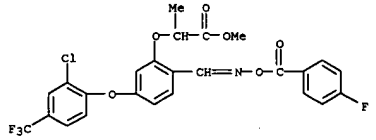


RN 128079-37-8 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[(2,4-dinitrobenzoyl)oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)

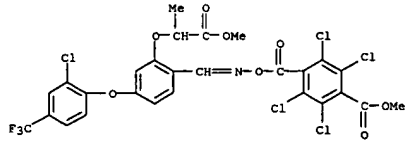
L27 ANSWER 12 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



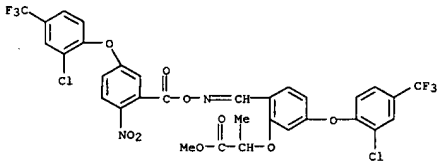
RN 128079-38-9 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[(4-fluorobenzoyl)oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



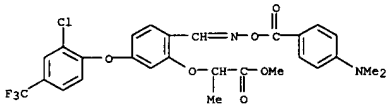
RN 128079-39-0 CAPLUS
CN Benzoic acid, 2,3,5,6-tetrachloro-4-[[[[[4-[2-chloro-4-(trifluoromethyl)phenoxy]-2-(2-methoxy-1-methyl-2-oxoethoxy)phenyl]methylene]amino]oxy]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)



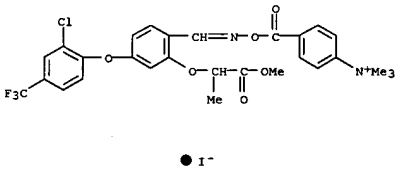
RN 128079-40-3 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitrobenzoyl]oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



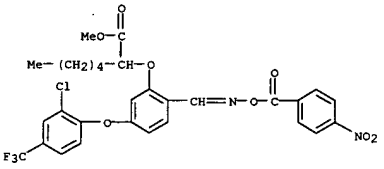
RN 128079-42-5 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[[4-(dimethylamino)benzoyl]oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



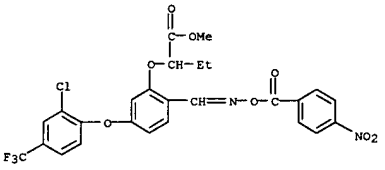
RN 128079-43-6 CAPLUS
CN Benzenaminium, 4-[[[[[4-[2-chloro-4-(trifluoromethyl)phenoxy]-2-(2-methoxy-1-methyl-2-oxoethoxy)phenyl]methylene]amino]oxy]carbonyl]-N,N,N-trimethyl-, iodide (9CI) (CA INDEX NAME)



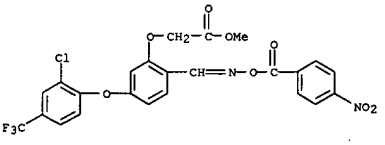
RN 128079-44-7 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[[4-(trifluoromethyl)benzoyl]oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



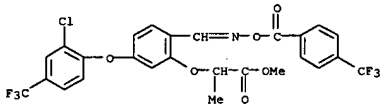
RN 128079-48-1 CAPLUS
CN Butanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[(4-nitrobenzoyl)oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



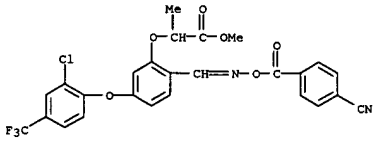
RN 128079-49-2 CAPLUS
CN Acetic acid, [5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[(4-nitrobenzoyl)oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



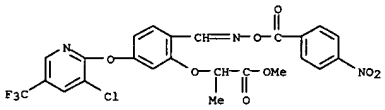
RN 128079-50-5 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[[(4-phenoxyphenoxy)carbonyl]oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



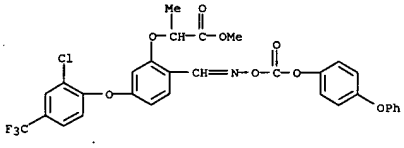
RN 128079-45-8 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[(4-cyanobenzoyl)oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



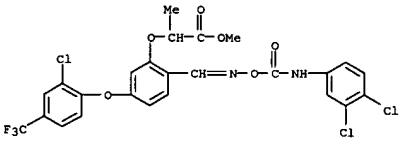
RN 128079-46-9 CAPLUS
CN Propanoic acid, 2-[5-[[3-chloro-5-(trifluoromethyl)-2-pyridinyl]oxy]-2-[[[(4-nitrobenzoyl)oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



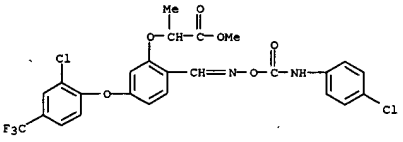
RN 128079-47-0 CAPLUS
CN Heptanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[(4-nitrobenzoyl)oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



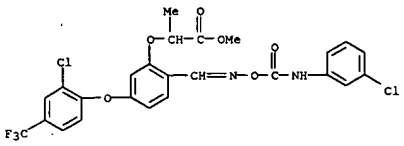
RN 128079-51-6 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[[[(3,4-dichlorophenyl)amino]carbonyl]oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



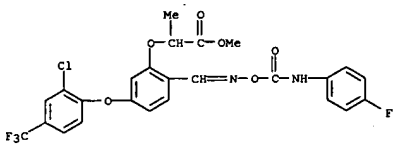
RN 128079-52-7 CAPLUS
CN Propanoic acid, 2-[2-[[[[[(4-chlorophenyl)amino]carbonyl]oxy]imino]methyl]-5-[2-chloro-4-(trifluoromethyl)phenoxy]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



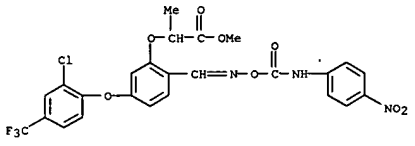
RN 128079-53-8 CAPLUS
CN Propanoic acid, 2-[2-[[[[[(3-chlorophenyl)amino]carbonyl]oxy]imino]methyl]-5-[2-chloro-4-(trifluoromethyl)phenoxy]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



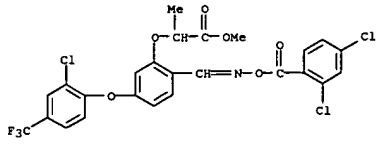
RN 128079-54-9 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[[[(4-fluorophenyl)amino]carbonyl]oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



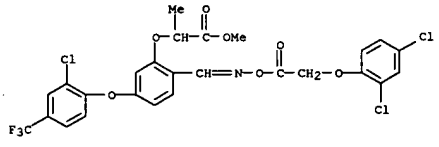
RN 128079-55-0 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[[[(4-nitrophenyl)amino]carbonyl]oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



RN 128079-57-2 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[(2,4-dichlorobenzoyl)oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



RN 128079-58-3 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[[(2,4-dichlorophenoxy)acetyl]oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



RN 128079-59-4 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[3-[4-[[3-chloro-5-(trifluoromethyl)-2-pyridinyl]oxy]phenoxy]-1-oxopropoxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)

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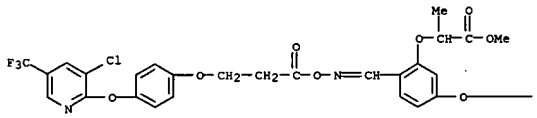

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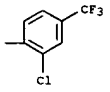
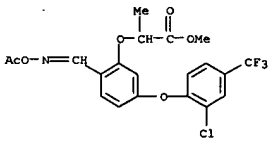


RN 128079-60-7 CAPLUS
CN Propanoic acid, 2-[2-[[(acetyloxy)imino]methyl]-5-[2-chloro-4-(trifluoromethyl)phenoxy]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



RN 128079-61-8 CAPLUS
CN Propanoic acid,
2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[1-oxo-3-[4-[[5-(trifluoromethyl)-2-pyridinyl]oxy]phenoxy]propoxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)

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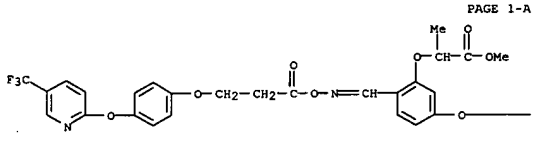

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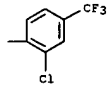
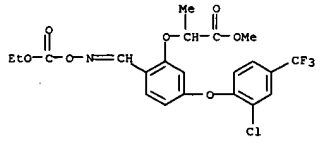
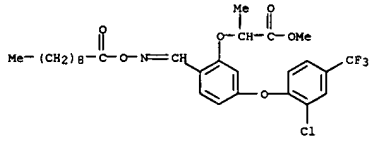


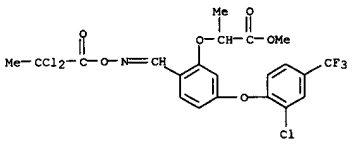
RN 128079-62-9 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[(ethoxycarbonyl)oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



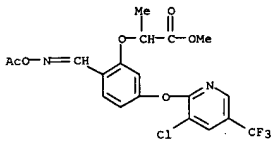
RN 128079-63-0 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[(1-oxodecyl)oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



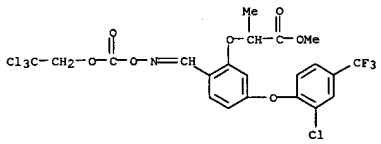
RN 128079-64-1 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[(2,2-dichloro-1-oxopropoxy)imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



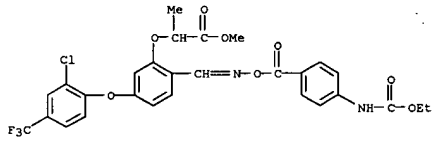
RN 128079-65-2 CAPLUS
CN Propanoic acid, 2-[2-[[(acetyloxy)imino]methyl]-5-[[3-chloro-5-(trifluoromethyl)-2-pyridinyl]oxy]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



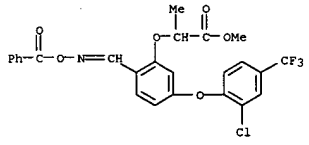
RN 128079-66-3 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[[(2,2,2-trichloroethoxy)carbonyl]oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



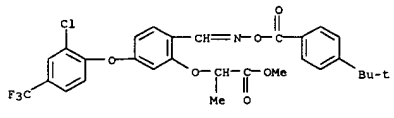
RN 128079-67-4 CAPLUS
CN Propanoic acid, 2-[2-[[[[(butylamino)carbonyl]oxy]imino]methyl]-5-[2-chloro-4-(trifluoromethyl)phenoxy]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



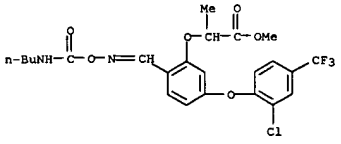
RN 128079-71-0 CAPLUS
CN Propanoic acid, 2-[2-[[(benzoyloxy)imino]methyl]-5-[2-chloro-4-(trifluoromethyl)phenoxy]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



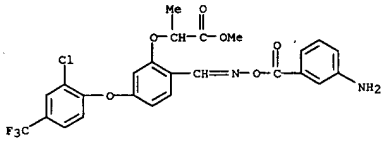
RN 128079-73-2 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[[4-(1,1-dimethylethyl)benzoyl]oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



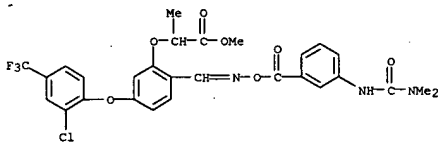
RN 128079-74-3 CAPLUS
CN Propanoic acid, 2-[2-[[[[4-[(chloroacetyl)amino]benzoyl]oxy]imino]methyl]-5-[2-chloro-4-(trifluoromethyl)phenoxy]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



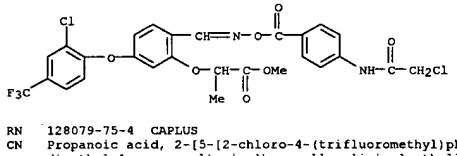
RN 128079-68-5 CAPLUS
CN Propanoic acid, 2-[2-[[[[(3-aminobenzoyl)oxy]imino]methyl]-5-[2-chloro-4-(trifluoromethyl)phenoxy]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



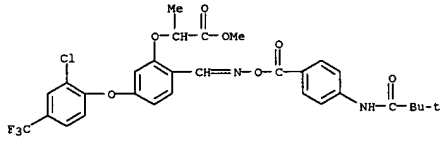
RN 128079-69-6 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[[3-[[(dimethylamino)carbonyl]amino]benzoyl]oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



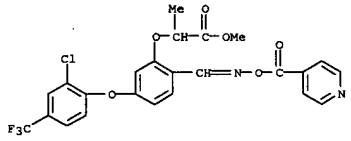
RN 128079-70-9 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[[4-[(ethoxycarbonyl)amino]benzoyl]oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



RN 128079-75-4 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[[4-[(2,2-dimethyl-1-oxopropyl)amino]benzoyl]oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



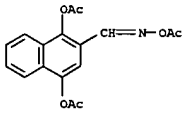
RN 128096-69-5 CAPLUS
CN Propanoic acid, 2-[5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-[[[(4-pyridinylcarbonyl)oxy]imino]methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



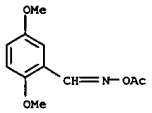
L27 ANSWER 13 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN
GI For diagram(s), see printed CA Issue.
AB The title compds. [I; R1, R4 = H, acyl, alkoxycarbonyl, alkylsulfonyl, dialkylcarbamoyl, alkoxyalkyl, alkyl; R2 = cyano, CHO, N-acyloxyiminomethyl, substituted CONH2, acylalkyl, (CH2CH:CMeCH2)nH (n = 2-4), CH2CH:CMe2, acyloxyalkyl, alkoxycarbonylalkyl, (un)substituted alkylsulfonyl, SO3H, substituted OH or NH2, N-substituted CH2NH2, CO2H, R; R3 = H, alkyl, acyloxyalkyl, etc.], useful for wound healing and for treatment of delayed allergies, are prepared Thus, treatment of 1,4-naphthalenediol ditetrahydropyranyl ether (preparation given) with BuLi in Et2O followed by DMF gave, after deprotection, 2-formyl-1,4-dihydroxynaphthalene which was acetylated with Ac2O in pyridine to give 2-formyl-1,4-diacetoxynaphthalene. I inhibited 24.2-96.6% auricle edema in mice sensitized with oxazolone.
ACCESSION NUMBER: 1990:118481 CAPLUS
DOCUMENT NUMBER: 112:118481
TITLE: Preparation of 1,4-dihydroxynaphthalene derivatives for wound healing and for treatment of delayed allergies
INVENTOR(S): Imuda, Junichi; Ishitoku, Takeshi; Isayama, Shigeru; Furuya, Yoshiro; Takahashi, Katsuya; Ori, Aiichiro; Nakamura, Hideo; Motoyoshi, Satoru
PATENT ASSIGNEE(S): Mitsui Petrochemical Industries, Ltd., Japan; Dainippon Pharmaceutical Co., Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 47 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01203351	A2	19890816	JP 1988-25330	19880205
PRIORITY APPLN. INFO.:			JP 1988-25330	19880205

OTHER SOURCE(S): MARPAT 112:118481
IT **125499-32-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as allergy inhibitor and for wound healing)
RN 125499-32-3 CAPLUS
CN 2-Naphthalenecarboxaldehyde, 1,4-bis(acetyloxy)-, 2-(O-acetyloxime) (9CI) (CA INDEX NAME)



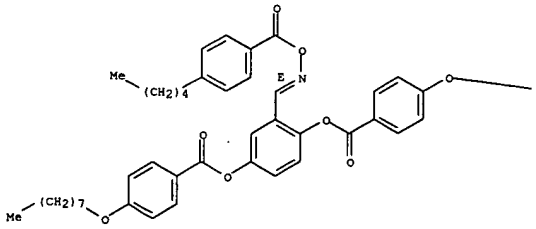
L27 ANSWER 14 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN
AB A new reagent, Me2NCH2CONMeOH (I), was developed for the selective cleavage of active esters under neutral conditions. Kinetic studies and applications of I are described.
ACCESSION NUMBER: 1989:552945 CAPLUS
DOCUMENT NUMBER: 111:152945
TITLE: N-Methyl-2-(dimethylamino)acetohydroxamic acid as a new reagent for the selective cleavage of active esters under neutral conditions
AUTHOR(S): Ono, Mitsunori; Itoh, Isamu
CORPORATE SOURCE: Ashigara Res. Lab., Fuji Photo Film Co., Ltd., Minami-Ashigara, 250 01, Japan
SOURCE: Tetrahedron Letters (1989), 30(2), 207-10
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:152945
IT **122913-67-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(ester cleavage of, in presence methyl(dimethylamino)acetohydroxamic acid)
RN 122913-67-1 CAPLUS
CN Benzaldehyde, 2,5-dimethoxy-, O-acetyloxime (9CI) (CA INDEX NAME)



L27 ANSWER 15 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN
AB The synthesis is described of 2-substituted hydroquinonebis(benzoates) which have large 2-substituents containing aromatic and other ring systems. Contrary to the general accepted opinion these large lateral substituents which cause remarkable deviations from the rodlike shape of the mols. do not prevent the liquid-crystalline properties, the compds. are nematic and smectic. The influence of different chemical groups on the liquid-crystalline properties was investigated systematically. The compds. tend to exhibit the glassy nematic state above room temperature This property may be used for the construction of thermoelectrooptic devices.
ACCESSION NUMBER: 1988:230022 CAPLUS
DOCUMENT NUMBER: 108:230022
TITLE: Thermotropic liquid-crystalline compounds with lateral long chain substituents. Part IX. Liquid-crystalline compounds with lateral aromatic branches
AUTHOR(S): Weissflog, W.; Demus, D.
CORPORATE SOURCE: VEB Laborchem., Leipzig-Lutzschena, DDR-7143, Ger. Dem. Rep.
SOURCE: Liquid Crystals (1988), 3(2), 275-84
CODEN: LICRE6; ISSN: 0267-8292
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **114391-76-3P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(liquid crystal, preparation and properties of)
RN 114391-76-3 CAPLUS
CN Benzoic acid, 4-(octyloxy)-, 2-[[[(4-pentylbenzoyl)oxy]imino]methyl]-1,4-phenylene ester, (E)- (9CI) (CA INDEX NAME)

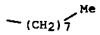
Double bond geometry as shown.

PAGE 1-A

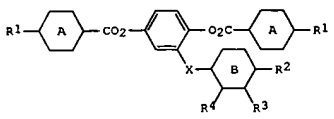


L27 ANSWER 15 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-B



L27 ANSWER 16 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN
GI



I

AB Liquid-crystalline 2-substituted-1,4-bis(4-substituted benzoyloxy)benzenes of formula I, where R1 = C1-12 alkyl or alkoxy; R2 = R1, (CH2)0-4CN, NO2, O2CC6H4R1, H, or Br; R3,R4 = H, alkyl, alkoxy, NO2, or CN; R2 + R3 = OCH2O; A = 1,4-phenylene or 1,4-cyclohexylene; B = A or pyridine; X = CO, R5C:NOOC, or COY; R5 = CnH2n (n = 0-4); Y = Z1(CH2)nZ2 (n = 0-10); Z1 = O, S, NR5, CHR5, CO, CH:CH, or N:CR5; and Z2 = Z1, OOC, or a single bond, can be used alone or mixed with each other or with other liquid-crystal or non-liquid-crystal materials.

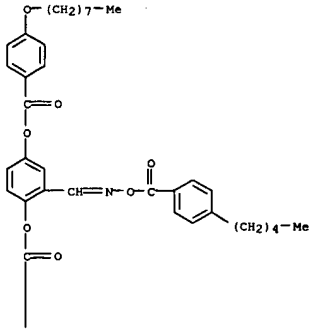
ACCESSION NUMBER: 1988:122081 CAPLUS
DOCUMENT NUMBER: 108:122081
TITLE: Glassy nematic liquid crystals as anisotropic solid optical materials for optical components and thermoelectrooptical storage displays
INVENTOR(S): Demus, Dietrich; Pelzl, Gerhard; Diele, Siegmar; Weissflog, Wolfgang; Wedler, Wolfgang
PATENT ASSIGNEE(S): Martin-Luther-Universitaet Halle-Wittenberg, Ger. Dem. Rep.
SOURCE: Ger. (East), 7 pp.
CODEN: GEXXA8
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 247227	A1	19870701	DD 1986-287593	19860305
DE 3703640	A1	19870910	DE 1987-3703640	19870206
CH 671233	A	19890815	CH 1987-560	19870212
GB 2188048	A1	19870923	GB 1987-4421	19870225
GB 2188048	B2	19900912		
JP 62212349	A2	19870918	JP 1987-48987	19870305
PRIORITY APPLN. INFO.:			DD 1986-287593 A	19860305

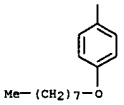
IT **113267-59-7**
RL: USES (Uses)
(glassy nematic liquid crystal, as anisotropic optical material)
RN 113267-59-7 CAPLUS
CN Benzoic acid, 4-(octyloxy)-, 2-[[[(4-pentylbenzoyl)oxy]imino]methyl]-1,4-phenylene ester (9CI) (CA INDEX NAME)

L27 ANSWER 16 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-A



PAGE 2-A

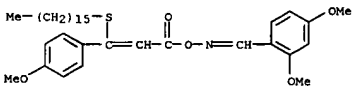


L27 ANSWER 17 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN
AB In the title process, the heating of imaging materials is carried out in the presence of the compound of the formula R1CX:CR2CO2N:CHR3 (R1, R2 = H, alkyl, cycloalkyl, alkenyl, alkynyl, aralkyl, aryl, heterocyclyl, carboxyl or its salt, halo, CN, alkylsulfonyl, arylsulfonyl, sulfamoyl, carbamoyl, alkoxycarbonyl, aryloxycarbonyl, alkylphosphoryl, arylphosphoryl, alkylphosphinyl, arylphosphinyl, alkylsulfinyl, arylsulfinyl, acyl, amino, acylamino, acyloxy, photog. useful group, R3 = aryl, heterocyclyl; X = photog. useful group; R1R2 combination may form a ring). The above compds. release development inhibitors with excellent timing.

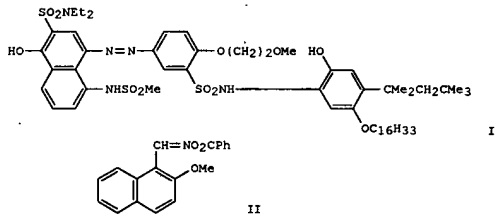
ACCESSION NUMBER: 1987:415617 CAPLUS
DOCUMENT NUMBER: 107:15617
TITLE: Imaging process involving heating step
INVENTOR(S): Sato, Kozo; Kato, Masatoshi; Kitaguchi, Hiroshi
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 19 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61267045	A2	19861126	JP 1985-106872	19850521
JP 05033780	B4	19930520		
PRIORITY APPLN. INFO.:			JP 1985-106872	19850521

IT **108859-53-6**
RL: USES (Uses)
(photothermog. development inhibitor-releasing compds.)
RN 108859-53-6 CAPLUS
CN Benzaldehyde, 2,4-dimethoxy-, O-[3-(hexadecylthio)-3-(4-methoxyphenyl)-1-oxo-2-propenyl]oxime (9CI) (CA INDEX NAME)



L27 ANSWER 18 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN
GI



I

II

AB Heat-developable photosensitive materials giving an image with a high signal-to-noise ratio, that is a high Dmax and a low Dmin, and a high d. are composed of a photosensitive gelatin-Ag halide emulsion layer, a dye-forming substance that upon reduction at a high temperature produces a diffusible dye, and an organic acid precursor with the structural unit -CH:NO2C- that is very stable at .ltorsim.50°, but frees an acid at temps. proceeding to development to neutralize the base and stop the development. Thus, a PET support was coated with a composition containing a gelatin-Ag(Br,I) emulsion 20, a gelatin-Ag benzotriazole emulsion 10, a dispersion of I 33 g, a 5% aqueous solution of p-C9H19C6H4O(CH2CH2O)10H 10, a 10% aqueous solution of H2NSO2NMe2 4, a gelatin dispersion of II 10 mL, and a solution of guanidine trichloroacetate 1.6 mL in EtOH 16 mL at 33μ (wet). After drying a gelatin protective layer was added. The resultant material was then imagewise exposed 10 s at 2000 lx with a W lamp, heated for 60 s on a 140° heating block, contacted with a wet receptor sheet, and heated 6 s at 80° to give a Dmax of 2.10 and a Dmin of 0.20 vs. 2.35 and 0.85, resp., for a II-free control.

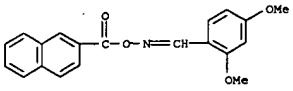
ACCESSION NUMBER: 1986:139353 CAPLUS
DOCUMENT NUMBER: 104:139353
TITLE: Heat-developing light-sensitive color material
INVENTOR(S): Kato, Masatoshi; Kitaguchi, Hiroshi
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd. , Japan
SOURCE: Ger. Offen., 90 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

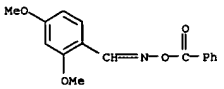
L27 ANSWER 18 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

DE 3508761	A1	19850919	DE 1985-3508761		19850312
JP 60192939	A2	19851001	JP 1984-48305		19840314
JP 04069775	B4	19921109			
US 4656126	A	19870407	US 1985-711885		19850314
PRIORITY APPLN. INFO.:			JP 1984-48305	A	19840314

IT **100906-54-5**
RL: USES (Uses)
(color diffusion-transfer photothermog. materials containing base-neutralizing acid precursor from, for improved image quality)
RN 100906-54-5 CAPLUS
CN Benzaldehyde, 2,4-dimethoxy-, O-(2-naphthalenylcarbonyl)oxime (9CI) (CA INDEX NAME)



L27 ANSWER 19 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L27 ANSWER 19 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN
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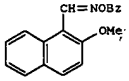


I

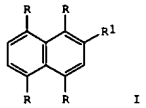
AB Organic acid precursors (R1CH:NO2C)nX [R1 = (un)substituted alkyl, cycloalkyl, aralkyl, alkenyl, (un)substituted aryl, heterocyclyl; X = (un)substituted alkyl, cycloalkyl, aralkyl, (un)substituted aryl, heterocycyl, or a mono-, di-, or trivalent group formed by combination of the above; n = 1-3], useful as agents to end development in a thermal photog. development process, were prepared Thus, 103.2 g 2-hydroxy-1-naphthaldehyde in DMF was etherified with 4-MeC6H4SO3Me and K2CO3 at 50-60° for 2 h to give 93.8 g 2-methoxy-1-naphthaldehyde, which (80 g) underwent oximation to give 85 g oxime. The oxime (70.3 g) was treated with 60% NaH in MeCN, and the resulting solution treated with BzCl at 10° to give 88 g acid precursor I. The reaction rate constant for cleavage of I to BzOH was 2.01/h at 100°, with T1/2 = 0.34 h.

ACCESSION NUMBER: 1986:50692 CAPLUS
DOCUMENT NUMBER: 104:50692
TITLE: Photographic material containing an acid precursor and
a procedure for producing a photographic image
INVENTOR(S): Kitaguchi, Hiroshi; Kato, Masatoshi
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd. , Japan
SOURCE: Ger. Offen., 40 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
DE 3442018	A1	19850530	DE 1984-3442018		19841116
JP 60108837	A2	19850614	JP 1983-216928		19831117
US 4670373	A	19870602	US 1984-672643		19841119
PRIORITY APPLN. INFO.:			JP 1983-216928	A	19831117

IT **99806-97-0**
RL: PRP (Properties)
(decomposition kinetics of)
RN 99806-97-0 CAPLUS
CN Benzaldehyde, 2,4-dimethoxy-, O-benzoyloxime (9CI) (CA INDEX NAME)

L27 ANSWER 20 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN
GI



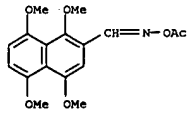
I

AB Alkoxynaphthalenes and their salts I [R = alkoxy; R1 = HOCH2, halomethyl, R2ON:CH (where R2 = H, alkyl), (CR3H)nR4 (where R3 = H, alkyl and R4 = CO2H, alkoxycarbonyl, cyano; n = 0, 1)], having inflammation inhibiting, antihypertensive, analgesic, antiallergic, and antihistaminic activities (no data), were prepared Thus, aqueous NaOH was added dropwise to a suspension of 1.8 g I (R = OMe; R1 = CHO) and 2.2 g Ag2O in CH2Cl2 and the resulting mixture heated 24 h at 60° to give 1 g I (R = OMe; R1 = CO2H).

ACCESSION NUMBER: 1985:471078 CAPLUS
DOCUMENT NUMBER: 103:71078
TITLE: Alkoxynaphthalene derivatives
PATENT ASSIGNEE(S): Otsuka Pharmaceutical Factory, Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 60036434	A2	19850225	JP 1983-145447	19830808
JP 03026177	B4	19910410		
PRIORITY APPLN. INFO.:			JP 1983-145447	19830808

OTHER SOURCE(S): CASREACT 103:71078
IT **97476-16-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 97476-16-9 CAPLUS
CN 2-Naphthalenecarboxaldehyde, 1,4,5,8-tetramethoxy-, O-acetyloxime (9CI) (CA INDEX NAME)



L27 ANSWER 20 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

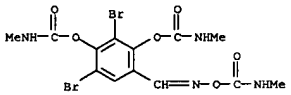
L27 ANSWER 21 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN

AB The oxime ethers Ar (SOn)mCX(:NOBA) (Ar = Ph, naphthyl, or heterocyclic radical; A = H, Cl-4 alkoxy, C2-4 alkenyloxy, Cl-4 alkylthio, etc.; B = Cl-4 alkylene or alkenylene, or direct bond; X = H, halo, alkylcarbamoyl, etc.; m = 0 or 1; n = 0, 1, or 2) are antidotes for known sulfonylurea herbicides. Thus, seed treatment with 2-FC6H4C(CN)(:NOCH2CN) [97627-47-9] (1 g/kg) protected corn by 50% against phytotoxicity from postemergence application of N-(2-methylbenzoylsulfonyl)-N'-(4-difluoromethoxy-6-methyl)pyrimidin-2-ylurea (62 g/ha), in pot expts.

ACCESSION NUMBER: 1985:466781 CAPLUS
DOCUMENT NUMBER: 103:66781
TITLE: Selectively active herbicides containing sulfonyl urea
as the active herbicidal agent as well as an antagonistically active oxime ether and their use for controlling weeds in food plant crops
INVENTOR(S): Gerber, Hans Rudolf; Bellucci, Sergio
PATENT ASSIGNEE(S): Ciba-Geigy A.-G. , Switz.
SOURCE: Eur. Pat. Appl., 50 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

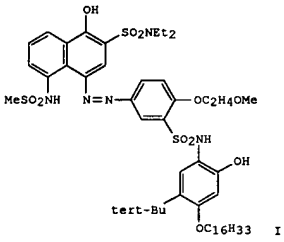
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 144283	A1	19850612	EP 1984-810470	19840928
R: BE, CH, DE, FR, GB, IT, LI, NL				
JP 60094902	A2	19850528	JP 1984-209016	19841004
PRIORITY APPLN. INFO.:			CH 1983-5389 A	19831004

IT **75409-11-9**
RL: BIOL (Biological study)
(as antidote, for sulfonylurea herbicides)
RN 75409-11-9 CAPLUS
CN Benzaldehyde, 3,5-dibromo-2,4-bis[[(methylamino)carbonyl]oxy]-, 1-[O-[(methylamino)carbonyl]oxime] (9CI) (CA INDEX NAME)

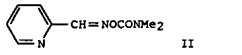


L27 ANSWER 22 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN

GI



I



II

AB A photog. material which forms low-fog storage-stable dye images by heating consists of ≥1 Ag halide emulsion, a binder, a dye-releasing redox compound, and a base precursor RCH:NOCONR1R2 (R = alkyl, cycloalkyl, alkenyl, aryl, aralkyl, acyl, heterocyclyl; R1, R2 = H, alkyl, cycloalkyl, aralkyl, or RR1 together can form a ring, or NRR1 may form an imino group by a double bond. Thus, a poly(ethylene terephthalate) support was coated with a composition containing a Ag(Br,I) emulsion 25, a dye-releasing redox compound dispersion (containing I 5, Na bis(2-ethylhexyl) sulfosuccinate 0.5, tricresyl phosphate 5, 10% aqueous gelatin 100 g, EtOAc 30 mL) 33 g, a 5% aqueous solution of C9H19C6H4-p-O(CH2CH2O)10H 10, a 10% aqueous solution of H2NSO2NMe2 4 mL, and a solution containing the base precursor II 2.5 g in EtOH 20 mL, to a wet thickness of 30 μm, dried, imagewise exposed to 2000 lx for 10 s using W lamp, heated 10 s to 140°, contacted with a H2O-wetted image receiver (consisting of a polyester support containing dispersed TiO2 and a gelatin layer of Me acrylate-N,N,N-trimethyl-N-vinylbenzylammonium chloride copolymer), and heated 6 s at 80°. After separation of the elements a neg. magenta image was obtained on the receiver whch had a Dmax and Dmin of 2.05 and 0.2, resp., vs. 0.03 and 0.03, resp., for a II-free control.

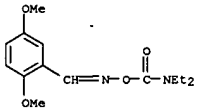
ACCESSION NUMBER: 1985:70099 CAPLUS
DOCUMENT NUMBER: 102:70099
TITLE: Heat-developable color photographic materials
INVENTOR(S): Hirai, Hiroyuki; Kawata, Ken

L27 ANSWER 22 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

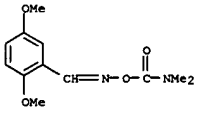
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd. , Japan
SOURCE: Eur. Pat. Appl., 61 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 118078	A2	19840912	EP 1984-101801	19840221
EP 118078	A3	19841128		
EP 118078	B1	19880107		
R: DE, FR, GB, NL				
JP 59157637	A2	19840907	JP 1983-31614	19830225
JP 02045180	B4	19901008		
US 4499180	A	19850212	US 1984-583913	19840227
PRIORITY APPLN. INFO.:			JP 1983-31614 A	19830225

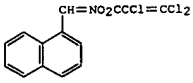
IT **93369-33-6P 93369-34-7P**
RL: PREP (Preparation)
(preparation of, for heat-developable color photog. materials)
RN 93369-33-6 CAPLUS
CN Benzaldehyde, 2,5-dimethoxy-, O-[(diethylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



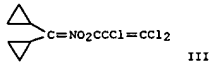
RN 93369-34-7 CAPLUS
CN Benzaldehyde, 2,5-dimethoxy-, O-[(dimethylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



L27 ANSWER 23 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN
GI



II



III

AB Cl2C:CClCO2N:CRR1 (I) (R,R1 = H, lower alkyl, benzyl, cycloalkyl, naphthyl, aryl, etc.) were prepared and shown, in some cases, to be more effective fungicides than kilazin P. Thus, 100 mL PhMe solution containing 40 g Cl2C:CClCOCl were added at ≤20° to 30 g PhCH:NOH and 26 g Et3N in 400 mL PhMe, and the mixture was heated 2 h at 50° to give 58 g I (R = Ph, R1 = H). Among 39 other I prepared were I [R,R1 = Me,Me; Me,Et; (RR1=) cyclohexylidene], the naphthyl analog II, and the dicyclopropyl analog III.

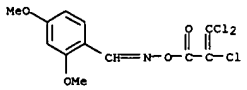
ACCESSION NUMBER: 1984:610740 CAPLUS
DOCUMENT NUMBER: 101:210740
TITLE: Trichloroacryloyl oxime derivatives
INVENTOR(S): Yamada, Yasuo; Saito, Junichi; Gotoh, Toshio; Katsumata, Osamu; Sakawa, Shinji
PATENT ASSIGNEE(S): Nihon Tokushu Noyaku Seizo K. K. , Japan
SOURCE: Eur. Pat. Appl., 34 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 112524	A1	19840704	EP 1983-112276	19831207
EP 112524	B1	19860528		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL				
JP 59110665	A2	19840626	JP 1982-220165	19821217
US 4581365	A	19860408	US 1983-557688	19831202
IL 70443	A1	19870130	IL 1983-70443	19831214
BR 8306913	A	19840724	BR 1983-6913	19831215
ZA 8309329	A	19840829	ZA 1983-9329	19831215
DK 8305810	A	19840618	DK 1983-5810	19831216
AU 8322504	A1	19840621	AU 1983-22504	19831219

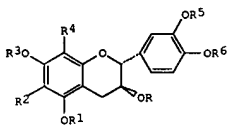
PRIORITY APPLN. INFO.: JP 1982-220165 A 19821217

OTHER SOURCE(S): CASREACT 101:210740
IT **93033-55-7P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as fungicide)
RN 93033-55-7 CAPLUS
CN Benzaldehyde, 2,4-dimethoxy-, O-(2,3,3-trichloro-1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)

L27 ANSWER 23 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L27 ANSWER 24 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN
GI



I

AB Cyanidanols I [R = H, (un)substituted hydrocarbon, acyl, carbamoyl; R1, R3, R5, R6 = H, (un)substituted hydrocarbon; R5R6 = CH2; R2, R4 = H, (un)substituted hydrocarbon, heterocyclic, halogen, CHO, (un)substituted CO2H, OH, SH, sulfamoyl, acyl, amino] were prepared Thus I (R = R1 = R3 = R5 = R6 = CH2Ph, R2 = R4 = H) was converted to its 8-formyl derivative which was subjected to Grignard reaction with EtBr to give I (R = R1 = R3 = R5 = R6 = CH2Ph, R2 = H, R4 = CHEtOH). Hydrogenation of the latter compound on Pd-C gave I (R = CH2Ph, R1-R3 = R5 = R6 = H, R4 = Pr) which had an ED50 against acute galactosamine hepatitis of 118.5 μmoles/kg orally in rats and 25 mg/kg i.p. in rats gave 56.1% inhibition of D-galactosamine edema.

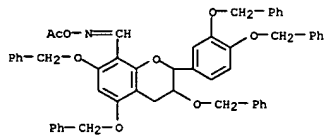
ACCESSION NUMBER: 1984:209512 CAPLUS
DOCUMENT NUMBER: 100:209512
TITLE: Pharmaceutical preparation containing (+)-cyanidan-3-ol derivatives, and use thereof
INVENTOR(S): Ballenegger, Marc Ernest; Rimbault, Christian Gerard; Albert, Alban Imre; Weith, Andre Jean; Courbat, Pierre; Tyson, Robert Graham; Palmer, Derek Reginald; Thompson, David George
PATENT ASSIGNEE(S): Zyma S. A., Switz.
SOURCE: Eur. Pat. Appl., 140 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 96007	A2	19831207	EP 1983-810222	19830526
EP 96007	A3	19840104		
EP 96007	B1	19870729		
R: AT, BE, CH, DE, FR, IT, LI, LU, NL, SE				
GB 2122608	A1	19840118	GB 1983-12765	19830510
GB 2122608	B2	19851002		
AT 28641	E	19870815	AT 1983-810222	19830526
FI 8301926	A	19831202	FI 1983-1926	19830530
ZA 8303908	A	19840125	ZA 1983-3908	19830530
ES 522814	A1	19850916	ES 1983-522814	19830530
CA 1234103	A1	19880315	CA 1983-429160	19830530
DK 8302452	A	19831202	DK 1983-2452	19830531
NO 8301950	A	19831202	NO 1983-1950	19830531
AU 8315255	A1	19831208	AU 1983-15255	19830531
AU 568301	B2	19871224		
JP 58219177	A2	19831220	JP 1983-96840	19830531
HU 31165	O	19840428	HU 1983-1943	19830531
DD 210687	A5	19840620	DD 1983-251542	19830531
IL 68832	A1	19880630	IL 1983-68832	19830531
ES 536423	A1	19870416	ES 1984-536423	19841001
US 4644011	A	19870217	US 1985-754181	19850709

PRIORITY APPLN. INFO.: GB 1982-15867 A 19820601
EP 1983-810222 A 19830526
US 1983-499647 A1 19830531

L27 ANSWER 24 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

OTHER SOURCE(S): CASREACT 100:209512
IT **89385-95-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dehydration of)
RN 89385-95-5 CAPLUS
CN 2H-1-Benzopyran-8-carboxaldehyde, 2-[3,4-bis(phenylmethoxy)phenyl]-3,4-dihydro-3,5,7-tris(phenylmethoxy)-, O-acetyloxime, (2R-trans)- (9CI) (CA INDEX NAME)



L27 ANSWER 25 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN
GI For diagram(s), see printed CA Issue.
AB Approx. 300 oximes R1CR2:NOR3 (R1 = substituted Ph or heterocyclic radical; R2 = H, CH, halogen, alkyl, etc.; R3 = H, alkyl, haloalkyl, alkenyl, alkylsulfonyl, etc.) were prepared and tested as herbicidal antidotes. Thus, seed treatment with 10 ppm (I) [34646-95-2] protected rice against the phytotoxic effect of Metolachlor [51218-45-2], in pot expts.

ACCESSION NUMBER: 1982:540287 CAPLUS
Correction of: 1981:78439
DOCUMENT NUMBER: 97:140287
Correction of: 94:78439
TITLE: Oxime derivatives and their use in the protection of cultivated plants
INVENTOR(S): Lukaszczyk, Alfons; Martin, Henry; Diel, Peter J.; Fory, Werner; Gatzi, Karl; Kristinsson, Haukur; Muller, Beat; Muntwyler, Rene; Pachlatko, Johannes Paul; et al.
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: Eur. Pat. Appl., 72 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

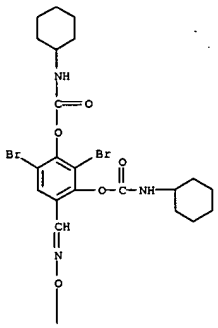
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 12158	A2	19800625	EP 1979-103212	19790830
EP 12158	A3	19800723		
EP 12158	B1	19840815		
R: AT, BE, CH, DE, FR, GB, IT, NL				
US 4347372	A	19820831	US 1979-70288	19790828
CS 210698	P	19820129	CS 1979-5915	19790830
CA 1164869	A1	19840403	CA 1979-334777	19790830
IL 58152	A1	19840531	IL 1979-58152	19790830
AT 8957	E	19840915	AT 1979-103212	19790830
AU 7950474	A1	19800320	AU 1979-50474	19790831
AU 541126	B2	19841220		
DD 146143	C	19810128	DD 1979-215309	19790831
JP 63017067	B4	19880412	JP 1979-112354	19790901
ZA 7904650	A	19800924	ZA 1979-4650	19790904
US 4388464	A	19830614	US 1981-232752	19810209
US 4715883	A	19871229	US 1982-423354	19820924

PRIORITY APPLN. INFO.:
CH 1978-9255 A 19780901
US 1979-70288 A3 19790828
EP 1979-103212 A 19790830
US 1981-232752 A3 19810209

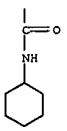
IT **75409-00-6P 75409-01-7P 75409-02-8P**
75409-03-9P 75409-04-0P 75409-05-1P
75409-06-2P 75409-07-3P 75409-08-4P
75409-09-5P 75409-10-8P 75409-11-9P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and herbicide-antidote activity of)

L27 ANSWER 25 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

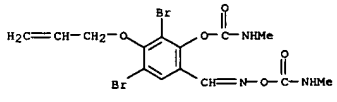
PAGE 1-A



PAGE 2-A

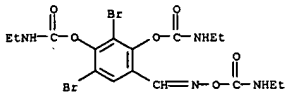


RN 75409-04-0 CAPLUS
CN Benzaldehyde, 3,5-dibromo-2-[[(methylamino)carbonyl]oxy]-4-(2-propenyloxy)-, 1-[O-[(methylamino)carbonyl]oxime] (9CI) (CA INDEX NAME)

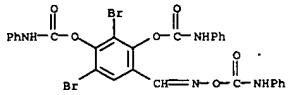


RN 75409-05-1 CAPLUS

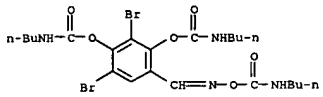
L27 ANSWER 25 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 75409-00-6 CAPLUS
CN Carbamic acid, ethyl-, 2,4-dibromo-6-[[[[(ethylamino)carbonyl]oxy]imino]methyl]-1,3-phenylene ester (9CI) (CA INDEX NAME)



RN 75409-01-7 CAPLUS
CN Benzaldehyde, 3,5-dibromo-2,4-bis[[(phenylamino)carbonyl]oxy]-, 1-[O-[(phenylamino)carbonyl]oxime] (9CI) (CA INDEX NAME)

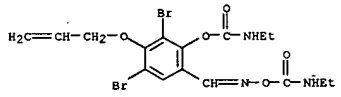


RN 75409-02-8 CAPLUS
CN Carbamic acid, butyl-, 2,4-dibromo-6-[[[[(butylamino)carbonyl]oxy]imino]methyl]-1,3-phenylene ester (9CI) (CA INDEX NAME)

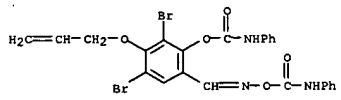


RN 75409-03-9 CAPLUS
CN Carbamic acid, cyclohexyl-, 2,4-dibromo-6-[[[[(cyclohexylamino)carbonyl]oxy]imino]methyl]-1,3-phenylene ester (9CI) (CA INDEX NAME)

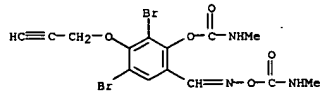
L27 ANSWER 25 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN Carbamic acid, ethyl-, 2,4-dibromo-6-[[[[(ethylamino)carbonyl]oxy]imino]methyl]-3-(2-propenyloxy)phenyl ester (9CI) (CA INDEX NAME)



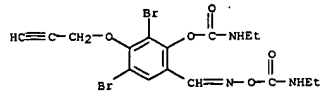
RN 75409-06-2 CAPLUS
CN Benzaldehyde, 3,5-dibromo-2-[[(phenylamino)carbonyl]oxy]-4-(2-propenyloxy)-, 1-[O-[(phenylamino)carbonyl]oxime] (9CI) (CA INDEX NAME)



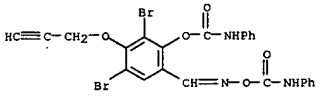
RN 75409-07-3 CAPLUS
CN Benzaldehyde, 3,5-dibromo-2-[[(methylamino)carbonyl]oxy]-4-(2-propynyloxy)-, 1-[O-[(methylamino)carbonyl]oxime] (9CI) (CA INDEX NAME)



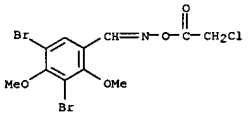
RN 75409-08-4 CAPLUS
CN Carbamic acid, ethyl-, 2,4-dibromo-6-[[[[(ethylamino)carbonyl]oxy]imino]methyl]-3-(2-propynyloxy)phenyl ester (9CI) (CA INDEX NAME)



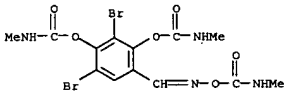
L27 ANSWER 25 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 75409-09-5 CAPLUS
CN Benzaldehyde,
3,5-dibromo-2-[[(phenylamino)carbonyl]oxy]-4-(2-propynyloxy)-
, 1-[O-[(phenylamino)carbonyl]oxime] (9CI) (CA INDEX NAME)



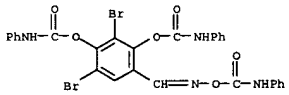
RN 75409-10-8 CAPLUS
CN Benzaldehyde, 3,5-dibromo-2,4-dimethoxy-, O-(chloroacetyl)oxime (9CI)
(CA
INDEX NAME)



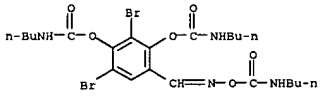
RN 75409-11-9 CAPLUS
CN Benzaldehyde, 3,5-dibromo-2,4-bis[[(methylamino)carbonyl]oxy]-,
1-[O-[(methylamino)carbonyl]oxime] (9CI) (CA INDEX NAME)



L27 ANSWER 26 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN Benzaldehyde, 3,5-dibromo-2,4-bis[[(phenylamino)carbonyl]oxy]-,
1-[O-[(phenylamino)carbonyl]oxime] (9CI) (CA INDEX NAME)

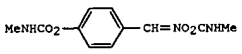


RN 75409-02-8 CAPLUS
CN Carbamic acid, butyl-,
2,4-dibromo-6-[[[[(butylamino)carbonyl]oxy]imino]me
thyl]-1,3-phenylene ester (9CI) (CA INDEX NAME)



RN 75409-03-9 CAPLUS
CN Carbamic acid, cyclohexyl-,
2,4-dibromo-6-[[[[(cyclohexylamino)carbonyl]ox
y]imino]methyl]-1,3-phenylene ester (9CI) (CA INDEX NAME)

L27 ANSWER 26 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN
GI



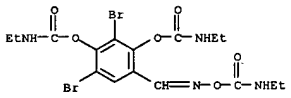
I

AB The oximes ArCX:NOQ (Ar = substituted Ph or heterocyclic radical; X = H, CH, halo, alkyl, etc.; Q = H, alkyl, haloalkyl, alkenyl, alkylsulfonyl, etc.) are herbicidal antidotes. Thus, seed treatment with 10 ppm I [34646-95-2] protected rice against the phytotoxic effect of Metolachlor [51218-45-2], in pot expts. The synthesis of the compds. is given.

ACCESSION NUMBER: 1981:78439 CAPLUS
DOCUMENT NUMBER: 94:78439
TITLE: Oxime derivatives and their use in the protection of cultivated plants
INVENTOR(S): Lukaszczyk, Alfons; Martin, Henry; Diel, Peter J.; Fory, Werner; Gatzi, Karl; Kristinsson, Haukur; Muller, Beat; Muntwyler, Rene; Pachlatko, Johannes Paul; et al.
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: Eur. Pat. Appl., 72 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 12158		19800625		
PRIORITY APPLN. INFO.:			CH 1978-9255	19780901

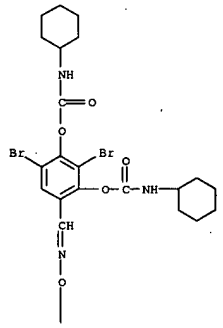
IT **75409-00-6P 75409-01-7P 75409-02-8P**
75409-03-9P 75409-04-0P 75409-05-1P
75409-06-2P 75409-07-3P 75409-08-4P
75409-09-5P 75409-10-8P 75409-11-9P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and herbicide-antidote activity of)
RN 75409-00-6 CAPLUS
CN Carbamic acid, ethyl-,
2,4-dibromo-6-[[[[(ethylamino)carbonyl]oxy]imino]me
thyl]-1,3-phenylene ester (9CI) (CA INDEX NAME)



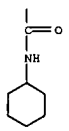
RN 75409-01-7 CAPLUS

L27 ANSWER 26 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

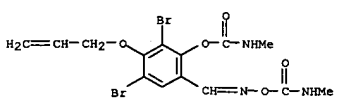
PAGE 1-A



PAGE 2-A

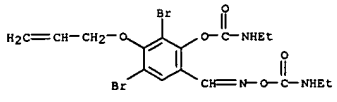


RN 75409-04-0 CAPLUS
CN Benzaldehyde,
3,5-dibromo-2-[[(methylamino)carbonyl]oxy]-4-(2-propenyloxy)-
, 1-[O-[(methylamino)carbonyl]oxime] (9CI) (CA INDEX NAME)

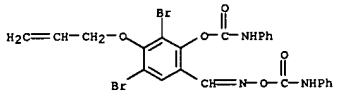


RN 75409-05-1 CAPLUS

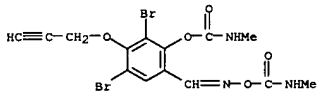
L27 ANSWER 26 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN Carbamic acid, ethyl-,
2,4-dibromo-6-[[[[(ethylamino)carbonyl]oxy]imino]me
thyl]-3-(2-propenyloxy)phenyl ester (9CI) (CA INDEX NAME)



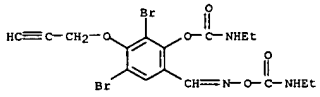
RN 75409-06-2 CAPLUS
CN Benzaldehyde,
3,5-dibromo-2-[[(phenylamino)carbonyl]oxy]-4-(2-propenyloxy)-
, 1-[O-[(phenylamino)carbonyl]oxime] (9CI) (CA INDEX NAME)



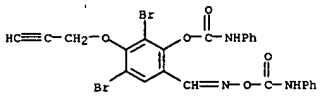
RN 75409-07-3 CAPLUS
CN Benzaldehyde,
3,5-dibromo-2-[[(methylamino)carbonyl]oxy]-4-(2-propynyloxy)-
, 1-[O-[(methylamino)carbonyl]oxime] (9CI) (CA INDEX NAME)



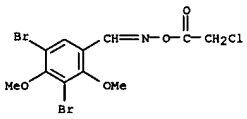
RN 75409-08-4 CAPLUS
CN Carbamic acid, ethyl-,
2,4-dibromo-6-[[[[(ethylamino)carbonyl]oxy]imino]me
thyl]-3-(2-propynyloxy)phenyl ester (9CI) (CA INDEX NAME)



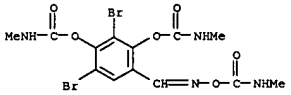
L27 ANSWER 26 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 75409-09-5 CAPLUS
CN Benzaldehyde,
3,5-dibromo-2-[[(phenylamino)carbonyl]oxy]-4-(2-propynyloxy)-
, 1-[O-[(phenylamino)carbonyl]oxime] (9CI) (CA INDEX NAME)



RN 75409-10-8 CAPLUS
CN Benzaldehyde, 3,5-dibromo-2,4-dimethoxy-, O-(chloroacetyl)oxime (9CI) (CA
INDEX NAME)



RN 75409-11-9 CAPLUS
CN Benzaldehyde, 3,5-dibromo-2,4-bis[[(methylamino)carbonyl]oxy]-,
1-[O-[(methylamino)carbonyl]oxime] (9CI) (CA INDEX NAME)



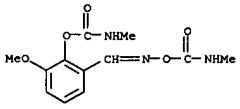
L27 ANSWER 27 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN
GI For diagram(s), see printed CA Issue.
AB Title compds. (I), used especially against Rhopalosiphum padi, Phaedon cochleariae, and Euscelis bilobatus, were prepared in 53.2-93.3% yield by reaction of MeNCO with the corresponding hydroxy-benzaldoximes. Thus, 2-hydroxybenzaldoxime in Et2O and MeNCO reacted 30 min at 10° in the presence of Et3N to give 67.8% I (R=H, O2CNHMe in position 2). Similarly prepared were 6 other I (R and position of O2CNHMe given): 5-Cl, 2; 3,5-Cl2, 2; 3-OMe, 2; H, 3; H, 4; and OMe, 4.

ACCESSION NUMBER:	1972:33961 CAPLUS
DOCUMENT NUMBER:	76:33961
TITLE:	Insecticidal and acaricidal hydroxybenzaldoxime bis(methylcarbamates)
INVENTOR(S):	Lorenz, Walter; Hammann, Ingeborg
PATENT ASSIGNEE(S):	Farbenfabriken Bayer A.-G.
SOURCE:	Ger. Offen., 21 pp. CODEN: GWXXBX
DOCUMENT TYPE:	Patent
LANGUAGE:	German
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
DE 2011182	A	19710923	DE 1970-2011182		19700310
PRIORITY APPLN. INFO.:			DE 1970-2011182	A	19700310

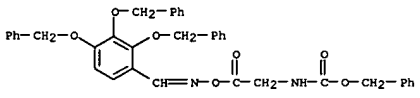
IT **34646-93-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 34646-93-0 CAPLUS
CN Benzaldehyde, 3-methoxy-2-[[(methylamino)carbonyl]oxy]-,
O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



L27 ANSWER 28 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN
AB 2,3,4-(HO)3C6H2CH2NHO2CCH2NH2.2HBr (I) is prepared from carbobenzoxyglycine and tritylhydroxylamine in 5 steps. In contrast to the corresponding isosteric 2,3,4-(HO)3C6H2CH2NHNHCOCH2NH2, I is not a decarboxylase inhibitor.

ACCESSION NUMBER:	1970:456389 CAPLUS
DOCUMENT NUMBER:	73:56389
TITLE:	Synthesis of O-glycyl-N(2,3,4-trihydroxybenzyl)hydroxylamine dihydrobromide
AUTHOR(S):	Hegedus, Balthasar; Krasso, A. F.
CORPORATE SOURCE:	Chem. Forschungsabt., F. Hoffmann-La Roche und Co. A.-G., Basel, Switz.
SOURCE:	Helvetica Chimica Acta (1970), 53(5), 959-63 CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE:	Journal
LANGUAGE:	German
OTHER SOURCE(S):	CASREACT 73:56389

IT **27916-68-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 27916-68-3 CAPLUS
CN Benzaldehyde, 2,3,4-tris(benzyloxy)-, O-(N-carboxyglycyl)oxime benzyl ester (8CI) (CA INDEX NAME)



L27 ANSWER 29 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN

AB The title compds. useful as insecticides, animal systemic parasiticides, herbicides, and foliage fungicides have the formula I. The intermediate 3-(diethoxyphosphinothioyl) benzaldehyde (II), n30D 1.5239 was prepared in 99.5% yield by refluxing 24.4 g. 3-hydroxybenzaldehyde, 37.8 g. O,O-diethylphos-phorochloridothioate, and 16.4 g. K2CO3 in 200 ml. Me Et ketone 4 hrs., the mixture poured into 300 ml. H2O and twice extracted with CHCl3, 7.5 g. Na2CO3.H2O added to a mixture of 27.4 g. II and 7.6 g. hydroxylamine hydrochloride in 300 ml. H2O at room temperature in 20 min., and the mixture stirred one hr. and extracted with C6H6 to give 68.3% 3-(diethoxyphosphinothioyl)benzaldoxime (III), n30D 1.5460. III (10 g.) in 10 ml. acetone was treated with excess MeNCO and poured into 200 ml. C6H6 to give 93.3% 3-(dieth-oxyphosphinothioyl) benzaldoxime methylcarbamate, n30D 1.5394. Similarly prepared in 96.9% yield was 4'-(diethoxyphosphino-thioyl)acetophenone oxime methylcarbamate. A mixture of 56.2 g. 4'-(diethoxyphosphinothioyl)acetophenone, 17.4 g. hydroxylamine hydrochloride, and 4 g. NaOH in 150 ml. 80% EtOH was refluxed 5 min., cooled, and acidified with concentrated HCl to give 93.5% 4'-(diethoxyphosphinothioyl)acetophenone oxime (IV), n30D 1.5393. A mixture of 10.0 g. IV, 3.2 g. AcCl, 4.1 g. Et3N, and 150 ml. C6H6 was refluxed one hr. to give 96.5% 4'-(diethoxy-phosphinothioyl)acetophenone oxime acetate, n30D 1.5279. A solution of 14.5 g. 4-(diethoxyphosphinothioyl)benzaldoxime. (V) in 50 ml. Et2O was added in 30 min. at 10° to 7 g. phosgene in 150 ml. Et2O, the mixture stirred one hr. at 15°, a solution of 17.4 g. morpholine in 10 ml. H2O added at <15°, and the mixture stirred two hrs. at room temperature and worked up to give 89.8% 4-(diethoxy-phosphinothioyl)benzaldoxime 4-morpholinecarboxylate, n30D 1.5423. Similarly 14.5 g. V, 7 g. phosgene, and 8.6 g. N,N-dimethylaniline treated with 6.1 g. ethanolamine and 10 ml. H2O at <15° gave 94.8% 4-(diethoxyphosphinothioyl)benzaldoxime (β-hydroxyethyl)carbamate (VI), n30D 1.5423. A solution of 11.6 g. N,N-diethylethylenediamine in 10 ml. H2O was added dropwise at <15° to VI in Et2O solution to give 51.8% 4-(diethoxyphos-phinothioyl)benzaldoxime 2-(diethylamino)ethyl carbamate, n30D 1.5310. These procedures were followed to obtain the tabulated I (X = S, p = position of phenyl substitution by R2C:NOR3 relative to P-containing group). The following VII were likewise prepared (R, R1, and n30D given): H, CONHMe, 1.5280; H, CONHBu, 1.5130; Me, CONHMe, 1.5243; Me, CONHPr-iso, 1.5109. The compds. prepared were tested as pre- and postemergent herbicides, as foliage fungicides, as insecticides, and for internal animal systematic activity.

ACCESSION NUMBER: 1969:430236 CAPLUS
DOCUMENT NUMBER: 71:30236
TITLE: (O-Carbamoyl oxime), phosphate, phosphonate, and phosphinate compositions and their utility as herbicides and pesticides
INVENTOR(S): Gutman, Arnold D.
PATENT ASSIGNEE(S): Stauffer Chemical Co.
SOURCE: S. African, 80 pp.
CODEN: SFXXAB

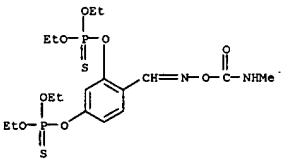
L27 ANSWER 29 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ZA 6803662		19681108		
DE 1768676			DE	
FR 1583911			FR	
GB 1229853			GB	
US 3652737		19720000	US	
US 3673181		19720000	US	
US 3681476		19720000	US	
US 3681478		19720000	US	
US 3681479		19720000	US	
US 3733375		19730000	US	
US 3749748		19730000	US	
US 3769419		19730000	US	
PRIORITY APPLN. INFO.:			US	19670616
			US	19680520

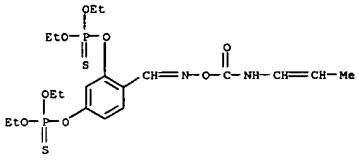
IT **22942-28-5P 22942-30-9P 22942-31-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 22942-28-5 CAPLUS
CN Phosphorothioic acid, O,O-diethyl ester, O,O-diester with β-resorcylaldehyde O-(methylcarbamoyl)oxime (8CI) (CA INDEX NAME)

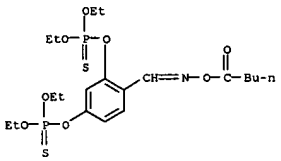


RN 22942-30-9 CAPLUS
CN Phosphorothioic acid, O,O-diethyl ester, O,O-diester with β-resorcylaldehyde O-(propenylcarbamoyl)oxime (8CI) (CA INDEX NAME)

L27 ANSWER 29 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 22942-31-0 CAPLUS
CN Phosphorothioic acid, O,O-diethyl ester, O,O-diester with β-resorcylaldehyde O-valeryloxime (8CI) (CA INDEX NAME)



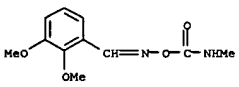
L27 ANSWER 30 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN

AB Carbaryl was applied topically, singly, and in combination with several series of adjuvants to the housefly to determine the role of the dioxole ring of methylenedioxyphenyl compds. in synergizing the carbamate insecticides. When the methylenedioxy moiety was replaced with methoxyl or methoxyl and hydroxyl groups, synergistic activity was greatly reduced or lost. Several 1,3-benzodioxans also failed to act as synergists. The integrity of the 1,2-methylenedioxy structure is essential for maximum potentiation of housefly toxicity of the carbamates, paralleling the case for pyrethrins synergism.

ACCESSION NUMBER: 1965:25221 CAPLUS
DOCUMENT NUMBER: 62:25221
ORIGINAL REFERENCE NO.: 62:4549f-g
TITLE: Influence of the methylenedioxyphenyl structure in synergism of a carbamate insecticide for house flies
AUTHOR(S): Moorefield, Herbert H.; Weiden, Mathias H. J.
CORPORATE SOURCE: Union Carbide Agr. Res. Sta., Clayton, NC
SOURCE: Contributions from Boyce Thompson Institute (1964), 22(8), 425-33
CODEN: CBTIAE; ISSN: 0006-8543
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **2815-70-5**, o-Veratraldehyde, O-(methylcarbamoyl)oxime
(as synergist for carbaryl, in housefly control)

RN 2815-70-5 CAPLUS
CN o-Veratraldehyde, O-(methylcarbamoyl)oxime (7CI, 8CI) (CA INDEX NAME)



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COST IN U.S. DOLLARS

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FULL ESTIMATED COST	170.25	2051.76

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-21.90	-72.17

FILE 'REGISTRY' ENTERED AT 16:15:45 ON 06 FEB 2005
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DICTIONARY FILE UPDATES: 4 FEB 2005 HIGHEST RN 825667-31-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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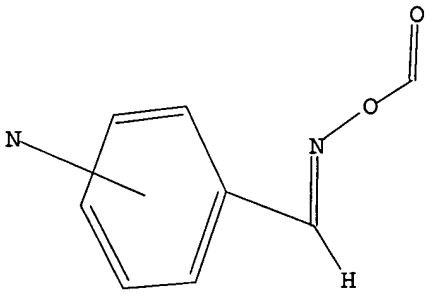
Uploading C:\Program Files\Stnexp\Queries\09734625.str

chain nodes :
1 2 3 4 5 6 13
ring nodes :
7 8 9 10 11 12
chain bonds :
1-2 1-4 1-11 2-3 3-6 5-6
ring bonds :
7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-2 2-3 3-6 5-6
exact bonds :
1-4 1-11
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS

L28 STRUCTURE UPLOADED

=> d query
L28 STR



Structure attributes must be viewed using STN Express query preparation.

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93.6% PROCESSED 1000 ITERATIONS 23 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 19400 TO 23320
PROJECTED ANSWERS: 194 TO 788

L29 23 SEA SSS SAM L28

=> s l28 full
FULL SEARCH INITIATED 16:16:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 20775 TO ITERATE

100.0% PROCESSED 20775 ITERATIONS 342 ANSWERS
SEARCH TIME: 00.00.02

L30 342 SEA SSS FUL L28

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 161.33 2213.09

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION

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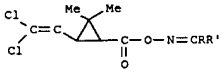
FILE COVERS 1907 - 6 Feb 2005 VOL 142 ISS 7
FILE LAST UPDATED: 4 Feb 2005 (20050204/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l30
L31 86 L30

=> d l31 1-86 abs ibib hitstr

L31 ANSWER 1 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
GI



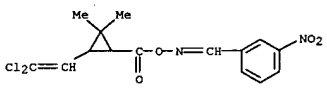
I

AB EI mass spectra of the title compds. (I; R = p-tert-butylphenyl, R'= MeS, EtS, PhCH2S, PhNH; etc) were measured. Fragmentation pathways include cleavage of the cyclopropane ring with migration of disubstituted methyleneamino moiety.

ACCESSION NUMBER: 2004:912549 CAPLUS
TITLE: Skeletal rearrangement of substituted benzaldoxime 3-(2,2-dichlorovinyl)-2,2-dimethyl cyclopropane carboxylates under EI-MS
AUTHOR(S): Xia, Yan; He, Shui-ji; Chen, Qi-fa; Zuo, Yu-min
CORPORATE SOURCE: Department of Chemistry, Nankai University, Tianjin, 300071, Peop. Rep. China
SOURCE: Chemical Research in Chinese Universities (2004), 20(5), 671-673
CODEN: CRCUED; ISSN: 1005-9040
PUBLISHER: Higher Education Press
DOCUMENT TYPE: Journal
LANGUAGE: English

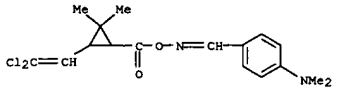
IT **205937-81-1 205937-83-3**
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(skeletal rearrangement of substituted benzaldoxime 3-(2,2-dichlorovinyl)-2,2-dimethyl cyclopropane carboxylates under EI-MS)

RN 205937-81-1 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[[3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropyl]carbonyl]oxime (9CI) (CA INDEX NAME)



RN 205937-83-3 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[[3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropyl]carbonyl]oxime (9CI) (CA INDEX NAME)

L31 ANSWER 1 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

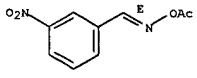
L31 ANSWER 2 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB In the title compound, C9H8N2O4, the 3-nitrobenzaldehyde oxime and acetyl group have a dihedral angle of 19.5(4)°. The acetyl carbonyl and 3-nitrobenzaldehyde oxime groups both adopt a trans configuration (E). In the crystal structure, mols. are linked by weak intermol. C-H...O interactions, forming a sheet-like structure parallel to the (303) plane. Crystallog. data are given.

ACCESSION NUMBER: 2004:622188 CAPLUS
DOCUMENT NUMBER: 142:65724
TITLE: (E)-3-Nitrobenzaldehyde O-acetyloxime
AUTHOR(S): Brito-Arias, Marco A.; Garcia-Baez, Efren V.; del Toro, Gustavo Valencia; Hoepfl, Herbert
CORPORATE SOURCE: Unidad Profesional Interdisciplinaria Biotecnologia, Barrio La Laguna Ticoman, Instituto Politecnico Nacional, Mexico City, DF 07340, Mex.
SOURCE: Acta Crystallographica, Section E: Structure Reports Online (2004), E60(8), o1451-o1452
CODEN: ACSEBH; ISSN: 1600-5368
URL: http://journals.iucr.org/e/graphics/htmlborder.gif
PUBLISHER: Blackwell Publishing Ltd.
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English

IT **808101-24-8P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

RN 808101-24-8 CAPLUS
CN Benzaldehyde, 3-nitro-, O-acetyloxime, [C(E)]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

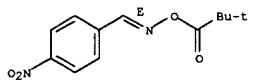
L31 ANSWER 3 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB The name of the second author, Wan Jin Jahng, was misspelled.

ACCESSION NUMBER: 2004:480085 CAPLUS
DOCUMENT NUMBER: 142:93231
TITLE: Elimination reactions of (E)-O-pivaloylbenzaldoximes. [Erratum to document cited in CA119:116591]
AUTHOR(S): Cho, Bong Rae; Jahng, Wan Jin; Je, Jong Tae; Bartsch, Richard A.
CORPORATE SOURCE: Dep. Chem., Korea Univ., Seoul, S. Korea
SOURCE: Journal of Organic Chemistry (2004), 69(14), 4870
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **149540-92-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(elimination reaction of, kinetics of (Erratum))

RN 149540-92-1 CAPLUS
CN Benzaldehyde, 4-nitro-, O-(2,2-dimethyl-1-oxopropyl)oxime, [C(E)]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L31 ANSWER 4 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN

AB ANHCO2B [A = dibenzofuranyl, dibenzothienyl, naphthyl, indolyl, fluorenyl, carbazolyl, alkoxyphenyl, etc.; a = 1, 2; R = (substituted) alkoxy, Ph, phenoxy; phenylalkoxy, pyridyloxy, pyridylalkoxy, NHCOalkyl, CONHalkyl; R1 = bond, aliphatic hydrocarbon; B = (substituted) alkyl, indolyl, benzofuranyl, benzothienyl, dibenzofuranyl, dibenzothienyl, fluorenyl, carbazolyl, naphthyl, quinolinyl, isoquinolinyl, N:CR2R3, (substituted) Ph, pyridinyl; R2 = H, halo, alkyl; R3 = alkyl, pyridyl, halo, (substituted) Ph], were prepared Thus, 4-heptyloxybenzoic acid (preparation given) in PhMe was treated with diphenylphosphoryl azide and the resultant mixture was stirred at r.t. for 10 min. and then at 105° for 60 min.; after the mixture was cooled to r.t., 3-pyridinealdoxime was added the mixture was stirred at r.t. for 10 min. and then at 80° for 1 h. to give 3-pyridinecarboxaldehyde, O-[[[4-(heptyloxy)phenyl]amino]carbonyl]oxime trifluoroacetate. The latter inhibited fatty acid amide hydrolase with IC50<10 nM.

ACCESSION NUMBER: 2003:633409 CAPLUS
DOCUMENT NUMBER: 139:179893
TITLE: Preparation of (hetero)aryl carbamates and oximes as fatty acid amide hydrolase inhibitors.
INVENTOR(S): Sit, Sing-Yuen; Xie, Kai; Deng, Hongfeng
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 104 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003065989	A2	20030814	WO 2003-US3222	20030204
WO 2003065989	A3	20040219		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003195226	A1	20031016	US 2003-357807	20030204
EP 1472215	A2	20041103	EP 2003-737600	20030204
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

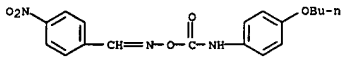
PRIORITY APPLN. INFO.: US 2002-355302P P 20020208
WO 2003-US3222 W 20030204

OTHER SOURCE(S): MARPAT 139:179893

IT **581071-01-4P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

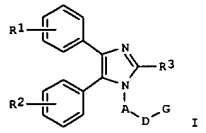
L31 ANSWER 4 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
(Uses)
(prepn. of (hetero)aryl carbamates and oximes as fatty acid amide hydrolase inhibitors)

RN 581071-01-4 CAPLUS
CN Benzaldehyde, 4-nitro-, O-[[(4-butoxyphenyl)amino]carbonyl]oxime (9CI) (CA INDEX NAME)

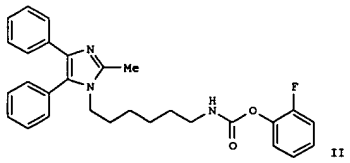


L31 ANSWER 5 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN

GI



I



II

AB Title compds. I [wherein R1 and R2 = independently H, alkyl, or halo; R3 = (cyclo)alkyl; A = alkylene or L; L = C6H4O-alkylene; D = CO2, CONG1, NHCO2, or NHCO2N:CG1; G = H, haloalkyl, (cyclo)alkyl, pyridyl, or (un)substituted Ph or (CH2)1-2Ph; G1 = H or (halo)alkyl; or AD is optionally interrupted with CHJ, ZC6H4, or Z(CH2)1-3; Z = O or S; J = alkyl or Ph; with provisos] were prepared as fatty acid amide hydrolase (FAAH) inhibitors. For example, cycloaddn. of benzil with AcONH4 and MeCHO in glacial AcOH gave 2-methyl-4,5-diphenyl-1H-imidazole (29%). Alkylation with Et 7-bromoheptanoate in the presence of NaH in DMF (72%) followed by saponification with NaOH in EtOH afforded 7-(2-methyl-4,5-diphenylimidazol-1-yl)heptanoic acid. Stepwise addition of the azide, N3PO(OPh)2, and 2-FC6H4OH to a suspension of the heptanoic acid in TEA and toluene produced the carbamate II (55%). The latter inhibited recombinant human FAAH with IC50 < 10 nM. In addition, II gave results similar to known analgesics in the in vivo rat formalin test (acute and chronic chemo-induced pain assay), the Hargreaves test (acute thermal pain assay), and the Chung model (neuropathic pain assay). Thus, I and their pharmaceutical compns. are useful for the treatment of pain, particularly neuropathic pain, psychomotor disorder, hypertension, cardiovascular disease, eating disorder, nausea, AIDS-related complex, glaucoma, inflammation, psoriasis or multiple sclerosis, and other conditions the treatment of which can be effected by inhibiting FAAH.

ACCESSION NUMBER: 2002:849426 CAPLUS
DOCUMENT NUMBER: 137:353021

L31 ANSWER 5 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
TITLE: Preparation of bisarylimidazolyl fatty acid amide hydrolase inhibitors for treatment of pain
INVENTOR(S): Sit, Sing-Yuen; Xie, Kai
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

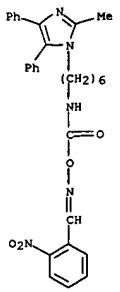
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002087569	A1	20021107	WO 2002-US12853	20020423
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002188009	A1	20021212	US 2002-128480	20020423
US 6562846	B2	20030513		
EP 1389107	A1	20040218	EP 2002-728952	20020423
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004532229	T2	20041021	JP 2002-584915	20020423

PRIORITY APPLN. INFO.: US 2001-286827P P 20010427
WO 2002-US12853 W 20020423

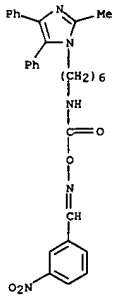
OTHER SOURCE(S): MARPAT 137:353021

IT **474430-34-7P**, 1-[[[[[[6-(2-Methyl-4,5-diphenyl-1H-imidazol-1-yl)hexyl]amino]carbonyl]oxy]imino]methyl]-2-nitrobenzene **474430-35-8P**, 1-[[[[[[6-(2-Methyl-4,5-diphenyl-1H-imidazol-1-yl)hexyl]amino]carbonyl]oxy]imino]methyl]-3-nitrobenzene **474430-36-9P**, 1-[[[[[[6-(2-Methyl-4,5-diphenyl-1H-imidazol-1-yl)hexyl]amino]carbonyl]oxy]imino]methyl]-4-nitrobenzene
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(FAAH inhibitor; preparation of bisarylimidazolyl fatty acid amide inhibitors for treatment of pain and other FAAH-related conditions)

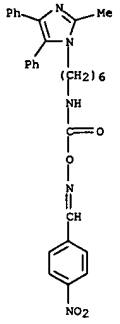
RN 474430-34-7 CAPLUS
CN Benzaldehyde, 2-nitro-, O-[[[6-(2-methyl-4,5-diphenyl-1H-imidazol-1-yl)hexyl]amino]carbonyl]oxime (9CI) (CA INDEX NAME)



RN 474430-35-8 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[[[6-(2-methyl-4,5-diphenyl-1H-imidazol-1-yl)hexyl]amino]carbonyl]oxime (9CI) (CA INDEX NAME)



RN 474430-36-9 CAPLUS
CN Benzaldehyde, 4-nitro-, O-[[[6-(2-methyl-4,5-diphenyl-1H-imidazol-1-yl)hexyl]amino]carbonyl]oxime (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

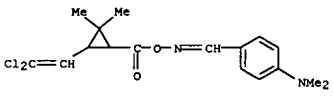
FORMAT

AB A series of compds. containing oxime-ester linkage in place of the ester linkage in pyrethroid ester were designed and prepared Bioassay data of insecticidal activities of these compds. on Ostrinia nubilalis (H.) and Culex pipiens (L.) are presented. Among them 4-dimethyaminobenzaldehyde oxime ester of 2,2,3,3-tetramethylcyclopropanecarboxylic acid and 4-dimethyamino benzaldehyde oxime ester of cyclopropanecarboxylic acid were found to be potent insecticide against Ostrinia nubilalis (H.). Structure-activity relationship of the compds. is discussed.

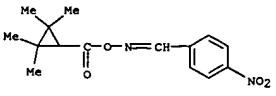
ACCESSION NUMBER: 2002:310814 CAPLUS
DOCUMENT NUMBER: 137:121038
TITLE: Synthesis and insecticidal activities of new pyrethroid acid oxime ester derivatives
AUTHOR(S): Ma, Jun'an; Huang, Runqiu; Chai, Youxin
CORPORATE SOURCE: Institute and State Key Laboratory of Elemento-organic Chemistry, Nankai University, Tianjin, 300071, Peop. Rep. China
SOURCE: Progress in Natural Science (2002), 12(4), 271-277
CODEN: PNASEA; ISSN: 1002-0071
PUBLISHER: Science in China Press
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:121038

IT **205937-83-3P 246532-24-1P 246532-31-0P 246532-32-1P 246532-33-2P 246532-34-3P 246532-35-4P 246532-36-5P 349450-90-4P 349450-91-5P 349450-92-6P 349450-93-7P 349450-94-8P 349450-95-9P 349450-96-0P 349450-97-1P 349450-98-2P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and insecticidal activities of)

RN 205937-83-3 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[[3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropyl]carbonyl]oxime (9CI) (CA INDEX NAME)

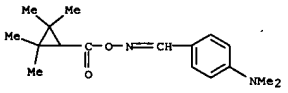


RN 246532-24-1 CAPLUS
CN Benzaldehyde, 4-nitro-, O-[(2,2,3,3-tetramethylcyclopropyl)carbonyl]oxime (9CI) (CA INDEX NAME)

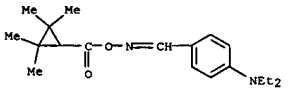


RN 246532-31-0 CAPLUS

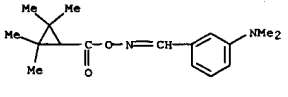
CN Benzaldehyde, 4-(dimethylamino)-, O-[(2,2,3,3-tetramethylcyclopropyl)carbonyl]oxime (9CI) (CA INDEX NAME)



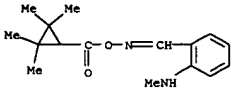
RN 246532-32-1 CAPLUS
CN Benzaldehyde, 4-(diethylamino)-, O-[(2,2,3,3-tetramethylcyclopropyl)carbonyl]oxime (9CI) (CA INDEX NAME)



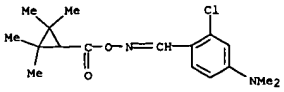
RN 246532-33-2 CAPLUS
CN Benzaldehyde, 3-(dimethylamino)-, O-[(2,2,3,3-tetramethylcyclopropyl)carbonyl]oxime (9CI) (CA INDEX NAME)



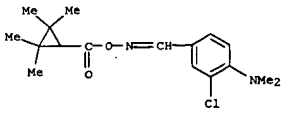
RN 246532-34-3 CAPLUS
CN Benzaldehyde, 2-(methylamino)-, O-[(2,2,3,3-tetramethylcyclopropyl)carbonyl]oxime (9CI) (CA INDEX NAME)



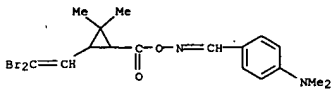
RN 246532-35-4 CAPLUS
CN Benzaldehyde, 2-chloro-4-(dimethylamino)-, O-[(2,2,3,3-tetramethylcyclopropyl)carbonyl]oxime (9CI) (CA INDEX NAME)



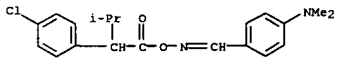
RN 246532-36-5 CAPLUS
CN Benzaldehyde, 3-chloro-4-(dimethylamino)-, O-[(2,2,3,3-tetramethylcyclopropyl)carbonyl]oxime (9CI) (CA INDEX NAME)



RN 349450-90-4 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[[3-(2,2-dibromoethenyl)-2,2-dimethylcyclopropyl]carbonyl]oxime (9CI) (CA INDEX NAME)

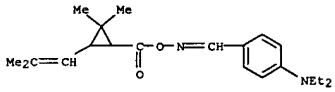


RN 349450-91-5 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[2-(4-chlorophenyl)-3-methyl-1-oxobutyl]oxime (9CI) (CA INDEX NAME)

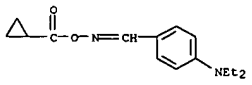


RN 349450-92-6 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[(2,2-dimethyl-3-(2-methyl-1-propenyl)cyclopropyl]carbonyl]oxime (9CI) (CA INDEX NAME)

propenyl)cyclopropyl]carbonyl]oxime (9CI) (CA INDEX NAME)

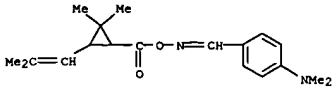


RN 349450-98-2 CAPLUS
CN Benzaldehyde, 4-(diethylamino)-, O-(cyclopropylcarbonyl)oxime (9CI) (CA INDEX NAME)

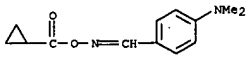


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

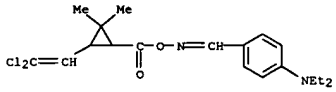
FORMAT



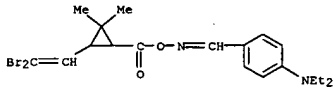
RN 349450-93-7 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(cyclopropylcarbonyl)oxime (9CI) (CA INDEX NAME)



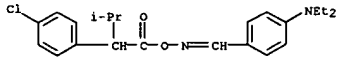
RN 349450-94-8 CAPLUS
CN Benzaldehyde, 4-(diethylamino)-, O-[[3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropyl]carbonyl]oxime (9CI) (CA INDEX NAME)



RN 349450-95-9 CAPLUS
CN Benzaldehyde, 4-(diethylamino)-, O-[[3-(2,2-dibromoethenyl)-2,2-dimethylcyclopropyl]carbonyl]oxime (9CI) (CA INDEX NAME)



RN 349450-96-0 CAPLUS
CN Benzaldehyde, 4-(diethylamino)-, O-[2-(4-chlorophenyl)-3-methyl-1-oxobutyl]oxime (9CI) (CA INDEX NAME)



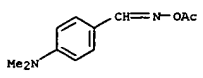
RN 349450-97-1 CAPLUS
CN Benzaldehyde, 4-(diethylamino)-, O-[[2,2-dimethyl-3-(2-methyl-1-

AB Fourteen novel title compds. 4-(RCOON:CH)C6H4N(CH3)2 (R = CH3, CH3CH2, ClCH2CH2, ClCH2, CH3CHCl, (CH3)2CH, (CH3)2CHCH2, CH2C(CH3), CH2:CHC(CH3)2CH2, 2,4-Cl2C6H3OCH(CH3), 4-ClC6H4OCH2, 4-(CH3)3CC6H4OCH(CH3), cyclopentyl) were synthesized. The bioassays indicated that title compds. (R = (CH3)2CH, (CH3)2CHCH2, 4-ClC6H4OCH2) possessed good insecticidal activity, compound showed significant fungicidal activity.

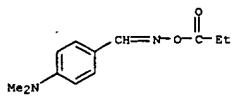
ACCESSION NUMBER: 2002:143944 CAPLUS
DOCUMENT NUMBER: 136:401508
TITLE: Synthesis and bioactivity of substituted benzaldoxime carboxylates. VI. Synthesis and bioactivity of 4-dimethylaminobenzaldoxime carboxylates
AUTHOR(S): Ma, Jun-an; Huang, Run-qiu; Chai, You-xin
CORPORATE SOURCE: State Key Lab. and Institute of Elemento-organic Chemistry, Nankai University, Tianjin, 300071, Peop. Rep. China
SOURCE: Yingyong Huaxue (2002), 19(2), 176-178
CODEN: YIHUED; ISSN: 1000-0518
PUBLISHER: Yingyong Huaxue Bianji Weiyuanhui
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 136:401508

IT **3986-36-5P 431046-75-2P 431046-76-3P 431046-77-4P 431046-78-5P 431046-79-6P 431046-80-9P 431046-81-0P 431046-82-1P 431046-83-2P 431046-84-3P 431046-85-4P 431046-86-5P 431047-48-2P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and bioactivity of substituted 4-dimethylaminobenzaldoxime carboxylates)

RN 3986-36-5 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-acetyloxime (9CI) (CA INDEX NAME)

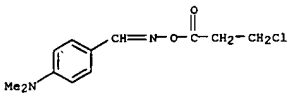


RN 431046-75-2 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(1-oxopropyl)oxime (9CI) (CA INDEX NAME)

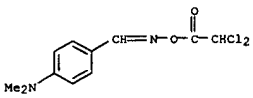


RN 431046-76-3 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(3-chloro-1-oxopropyl)oxime (9CI) (CA

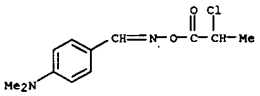
L31 ANSWER 7 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
INDEX NAME)



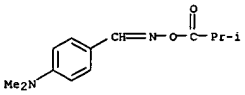
RN 431046-77-4 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(dichloroacetyl)oxime (9CI) (CA INDEX
NAME)



RN 431046-78-5 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(2-chloro-1-oxopropyl)oxime (9CI) (CA
INDEX NAME)

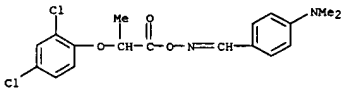


RN 431046-79-6 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(2-methyl-1-oxopropyl)oxime (9CI) (CA
INDEX NAME)

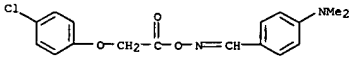


RN 431046-80-9 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(3-methyl-1-oxobutyl)oxime (9CI) (CA

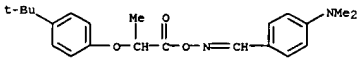
L31 ANSWER 7 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



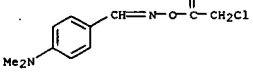
RN 431046-85-4 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[(4-chlorophenoxy)acetyl]oxime (9CI)
(CA INDEX NAME)



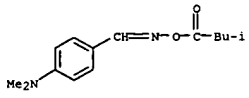
RN 431046-86-5 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[2-[4-(1,1-dimethylethyl)phenoxy]-1-
oxopropyl]oxime (9CI) (CA INDEX NAME)



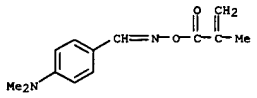
RN 431047-48-2 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(chloroacetyl)oxime (9CI) (CA INDEX
NAME)



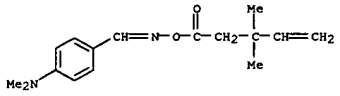
L31 ANSWER 7 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
INDEX NAME)



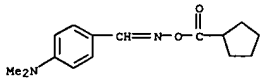
RN 431046-81-0 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(2-methyl-1-oxo-2-propenyl)oxime
(9CI)
(CA INDEX NAME)



RN 431046-82-1 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(3,3-dimethyl-1-oxo-4-pentenyl)oxime
(9CI) (CA INDEX NAME)



RN 431046-83-2 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(cyclopentylcarbonyl)oxime (9CI) (CA
INDEX NAME)



RN 431046-84-3 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[2-(2,4-dichlorophenoxy)-1-
oxopropyl]oxime (9CI) (CA INDEX NAME)

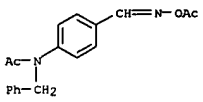
L31 ANSWER 8 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB The invention relates to a photopolymn. initiator of oxime ester for a photoresist composition, wherein the oxime is derivative of Ar1-C=N-OR1(H) (R1 = cycloalkanoyl, benzoyl, alkenoyl; Ar1 = aryl, aroyl). The photopolymn. initiator provides the alkali-developable light-sensitive photoresist composition, which shows the improved storageability, of the high resolution and the good storageability.

ACCESSION NUMBER: 2001:752026 CAPLUS
DOCUMENT NUMBER: 135:280493
TITLE: Photopolymerization initiator of oxime ester for light-sensitive photoresist composition
INVENTOR(S): Kunimoto, Kazuhiko; Oka, Hidetaka; Ohwa, Masaki; Tanabe, Junichi; Kura, Hisatoshi; Birbaum, Jean Luc
PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc.; Switz.
SOURCE: Fr. Demande, 171 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

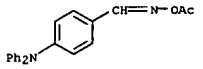
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2802528	A1	20010622	FR 2000-16306	20001214
TW 499411	B	20020821	TW 2000-89123924	20001110
NL 1016815	A1	20010618	NL 2000-1016815	20001206
NL 1016815	C2	20020514		
GB 2358017	A1	20010711	GB 2000-29793	20001207
GB 2358017	B2	20020313		
SE 2000004564	A	20020612	SE 2000-4564	20001211
SE 522774	C2	20040302		
US 2001012596	A1	20010809	US 2000-734625	20001212
JP 2001233842	A2	20010828	JP 2000-377671	20001212
IT 1319688	B1	20031023	IT 2000-MI2676	20001212
CA 2328376	AA	20010615	CA 2000-2328376	20001213
FI 2000002730	A	20010616	FI 2000-2730	20001213
DE 10061947	A1	20010621	DE 2000-10061947	20001213
ES 2177438	A1	20021201	ES 2000-2977	20001213
ES 2177438	B1	20041016		
DK 200001878	A5	20010616	DK 2000-1878	20001214
BE 1013872	A5	20021105	BE 2000-789	20001214
CN 1299812	A	20010620	CN 2000-135980	20001215
BR 2000006379	A	20010724	BR 2000-6379	20001215
PRIORITY APPLN. INFO.:			EP 1999-811160 A	19991215
			EP 2000-810629 A	20000717

IT **362624-53-1P 362624-79-1P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(light-sensitive color filter composition containing oxime esters used in optical imaging devices)
RN 362624-53-1 CAPLUS
CN Acetamide, N-[4-[[(acetyloxy)imino]methyl]phenyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

L31 ANSWER 8 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

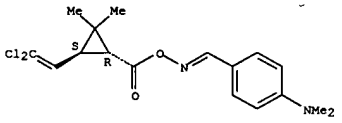


RN 362624-79-1 CAPLUS
CN Benzaldehyde, 4-(diphenylamino)-, O-acetyloxime (9CI) (CA INDEX NAME)



L31 ANSWER 9 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB Twelve of novel substituted benzaldehyde oxime ester of pyrethroid acids were synthesized, and their insecticidal activities and fungicidal activities were examined
ACCESSION NUMBER: 2001:276318 CAPLUS
DOCUMENT NUMBER: 135:88602
TITLE: Synthesis and bioactivity of substituted benzaldehyde oxime carboxylate (IV) synthesis and bioactivity of 4-dimethyl(ethyl)amine benzaldehyde oxime ester of pyrethroid acids
AUTHOR(S): Ma, Jun'an; Huang, Runqiu; Feng, Lei; Chai, Youxin
CORPORATE SOURCE: Institute of Elemento-organic Chemistry, Nankai University, Tianjin, 300071, Peop. Rep. China
SOURCE: Nongyaoxue Xuebao (1999), 1(3), 8-13
CODEN: NXOUAS; ISSN: 1008-7303
PUBLISHER: Nongyaoxue Xuebao Bianjibu
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 135:88602
IT **349450-99-3 349451-00-9 349451-01-0 349451-02-1**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(synthesis and bioactivity of substituted benzaldehyde oxime carboxylate - synthesis and bioactivity of 4-dimethyl(ethyl)amine benzaldehyde oxime ester of pyrethroid acids)
RN 349450-99-3 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[[(1R,3S)-3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropyl]carbonyl]oxime, rel- (9CI) (CA INDEX NAME)

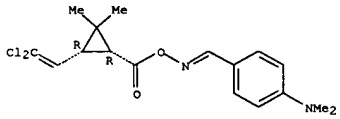
Relative stereochemistry.
Double bond geometry unknown.



RN 349451-00-9 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[[(1R,3R)-3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropyl]carbonyl]oxime, rel- (9CI) (CA INDEX NAME)

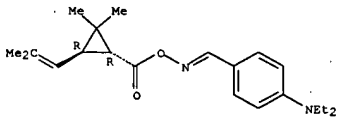
Relative stereochemistry.
Double bond geometry unknown.

L31 ANSWER 9 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



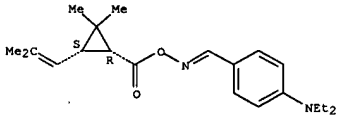
RN 349451-01-0 CAPLUS
CN Benzaldehyde, 4-(diethylamino)-, O-[[(1R,3R)-2,2-dimethyl-3-(2-methyl-1-propenyl)cyclopropyl]carbonyl]oxime, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



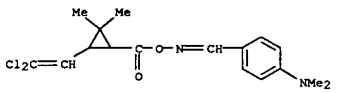
RN 349451-02-1 CAPLUS
CN Benzaldehyde, 4-(diethylamino)-, O-[[(1R,3S)-2,2-dimethyl-3-(2-methyl-1-propenyl)cyclopropyl]carbonyl]oxime, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

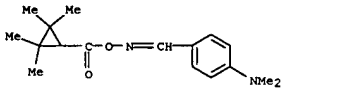


IT **205937-83-3P 246532-31-0P 246532-32-1P 349450-90-4P 349450-91-5P 349450-92-6P 349450-93-7P 349450-94-8P 349450-95-9P 349450-96-0P 349450-97-1P 349450-98-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and bioactivity of substituted benzaldehyde oxime carboxylate - synthesis and bioactivity of 4-dimethyl(ethyl)amine benzaldehyde oxime ester of pyrethroid acids)
RN 205937-83-3 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[[3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropyl]carbonyl]oxime (9CI) (CA INDEX NAME)

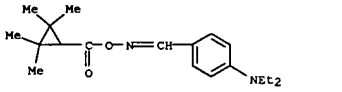
L31 ANSWER 9 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



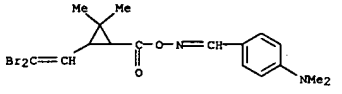
RN 246532-31-0 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[(2,2,3,3-tetramethylcyclopropyl)carbonyl]oxime (9CI) (CA INDEX NAME)



RN 246532-32-1 CAPLUS
CN Benzaldehyde, 4-(diethylamino)-, O-[(2,2,3,3-tetramethylcyclopropyl)carbonyl]oxime (9CI) (CA INDEX NAME)

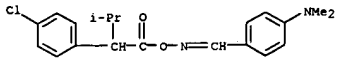


RN 349450-90-4 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[[3-(2,2-dibromoethenyl)-2,2-dimethylcyclopropyl]carbonyl]oxime (9CI) (CA INDEX NAME)

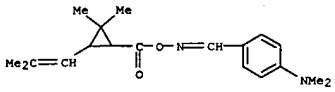


RN 349450-91-5 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[2-(4-chlorophenyl)-3-methyl-1-oxobutyl]oxime (9CI) (CA INDEX NAME)

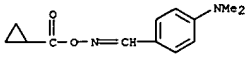
L31 ANSWER 9 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



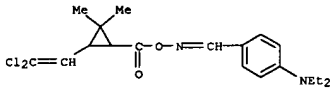
RN 349450-92-6 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[[2,2-dimethyl-3-(2-methyl-1-propenyl)cyclopropyl]carbonyl]oxime (9CI) (CA INDEX NAME)



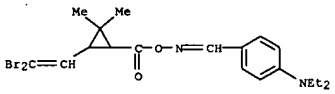
RN 349450-93-7 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(cyclopropylcarbonyl)oxime (9CI) (CA INDEX NAME)



RN 349450-94-8 CAPLUS
CN Benzaldehyde, 4-(diethylamino)-, O-[[3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropyl]carbonyl]oxime (9CI) (CA INDEX NAME)

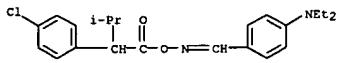


RN 349450-95-9 CAPLUS
CN Benzaldehyde, 4-(diethylamino)-, O-[[3-(2,2-dibromoethenyl)-2,2-dimethylcyclopropyl]carbonyl]oxime (9CI) (CA INDEX NAME)

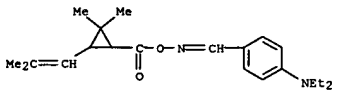


RN 349450-96-0 CAPLUS
CN Benzaldehyde, 4-(diethylamino)-, O-[2-(4-chlorophenyl)-3-methyl-1-

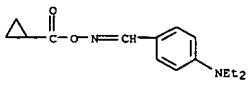
L31 ANSWER 9 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
oxobutyl]oxime (9CI) (CA INDEX NAME)



RN 349450-97-1 CAPLUS
CN Benzaldehyde, 4-(diethylamino)-, O-[[2,2-dimethyl-3-(2-methyl-1-propenyl)cyclopropyl]carbonyl]oxime (9CI) (CA INDEX NAME)

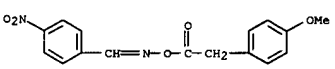


RN 349450-98-2 CAPLUS
CN Benzaldehyde, 4-(diethylamino)-, O-(cyclopropylcarbonyl)oxime (9CI) (CA INDEX NAME)



L31 ANSWER 10 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB A new safety catch linker for esters has been synthesized on polystyrene resin. This 2-tert-butoxyphenol resin may be acylated to give a relatively stable ester that will allow nucleophilic chemical without reaction at the linking ester group. Removal of the tert-Bu group with acid unmasks a highly reactive 2-hydroxyphenyl ester that reacts readily with nucleophiles to cause release of the product from the resin. This sequence has been exemplified by acylating the resin with various bromo acids, carrying out nucleophilic displacements with thiols, phenols, or amines, activating the ester with trifluoroacetic acid and cleaving from the resin with amines to give the (nucleophile) substituted carboxamides in high yield and purity. Kinetic studies with a model ester revealed half-lives for reaction with morpholine of 119 h for the tert-butoxyphenyl ester and 1 min for the corresponding phenol.

ACCESSION NUMBER: 2001:172610 CAPLUS
DOCUMENT NUMBER: 134:352969
TITLE: The Preparation of a New "Safety Catch" Ester Linker for Solid-Phase Synthesis
AUTHOR(S): Beech, Claire L.; Coope, John F.; Fairley, Gary; Gilbert, Philip S.; Main, Brian G.; Ple, Karen
CORPORATE SOURCE: AstraZeneca Pharmaceuticals Ltd., Macclesfield Cheshire, SK10 4TG, UK
SOURCE: Journal of Organic Chemistry (2001), 66(7), 2240-2245
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:352969
IT **339306-03-5DP**, polymer-supported
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(rate of reaction of polymer-supported esters with morpholine)
RN 339306-03-5 CAPLUS
CN Benzaldehyde, 4-nitro-, O-[(4-methoxyphenyl)acetyl]oxime (9CI) (CA INDEX NAME)

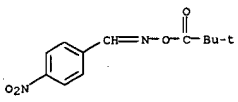


REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

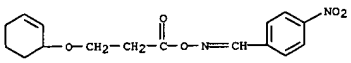
L31 ANSWER 11 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB Photolyses of aldoxime esters, containing a considerable range of alkyl groups, lead to cleavage of their N-O bonds and formation of aryliminyl and alkyl radicals. The process was found to be favored by 4-methoxyacetophenone as a photosensitizer and by methoxy substituents in the aryl rings. 4-Nitro- and pentafluoro-substitutions of the aryl rings were, on the other hand, deleterious. The intermediate iminyl radicals, together with primary, secondary and tertiary alkyl radicals were characterized by 9 GHz EPR spectroscopy. Cyclopropyl, CF3, and CCl3 radicals were probably also formed, but were too reactive for direct EPR spectroscopic detection. Photosensitized reaction of benzophenone oxime O-nonanoyl ester produced the diphenylmethaniminoxyl, as well as the expected n-octyl and iminyl radicals. This indicated that O-C bond scission accompanied O-N scission for this ketoxime ester. At higher temps. the C-centered radicals added to the starting oxime esters to produce alkoxyaminyl radicals that were also spectroscopically detected in some cases. No evidence for abstraction of the iminyl hydrogen by tert-butoxyl radicals was obtained. Instead, the t-BuO• radicals added to the C:N double bonds of the oxime esters. Similarly, chlorine abstraction from alkylbenzohydroximoyl chlorides by trimethyltin radicals did not take place. Preparative scale expts. with oxime esters containing suitably unsatd. alkyl groups showed that good yields of cyclised products could be obtained in the presence of the photosensitizer. This process constitutes a general method by which carboxylic acids or acid chlorides can be converted into alkyl radicals and hence to cyclized deriva.

ACCESSION NUMBER: 2000:832599 CAPLUS
DOCUMENT NUMBER: 134:178233
TITLE: Exploitation of aldoxime esters as radical precursors in preparative and EPR spectroscopic roles
AUTHOR(S): McCarroll, Andrew J.; Walton, John C.
CORPORATE SOURCE: University of St. Andrews, School of Chemistry, St Andrews, Fife, KY16 9ST, UK
SOURCE: Perkin 2 (2000), (12), 2399-2409
CODEN: PRKTFO; ISSN: 1470-1820
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:178233
IT **326853-02-5P 326853-03-6P**
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(attempted photolysis; preparative and ESR studies of the photolysis of aldoxime esters as radical precursors)
RN 326853-02-5 CAPLUS
CN Benzaldehyde, 4-nitro-, O-(2,2-dimethyl-1-oxopropyl)oxime (9CI) (CA INDEX NAME)

L31 ANSWER 11 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

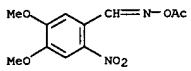


RN 326853-03-6 CAPLUS
CN Benzaldehyde, 4-nitro-, O-[3-(2-cyclohexen-1-yloxy)-1-oxopropyl]oxime (9CI) (CA INDEX NAME)



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

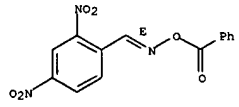
L31 ANSWER 12 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB The synthesis of caged NADP analogs 18, 19, and 20 has been accomplished by utilizing the transglycosidase activity of solubilized NAD glycohydrolase (porcine brain) to incorporate caged nicotinamides 2, 3, and 4 into NADP. The synthesis of several nicotinamides modified at the carboxamide with o-nitrobenzyl photolabile groups is demonstrated as well as their potential for enzymic transglycosidation. These results further demonstrate the feasibility of direct enzymic transglycosidation of sterically hindered substrates into NAD(P), although high nicotinamide analog water solubility was found to be a necessary trait for yield enhancement
with certain analogs. Caged analogs were surveyed under aqueous conditions
for net NADP photorelease, while the UV and fluorescent properties of both
analogs and their photobyproducts were assessed for compatibility with systems that rely on optical monitoring of enzyme activity. A highly water-soluble α-methyl-o-nitrobenzyl group 8 was developed for the synthesis of 20 in order to enhance net NADP photorelease. Compound 20 demonstrated a high 75% net NADP photoreleased without substantial UV optical blackening or fluorescent byproducts. Analogs 18 and 19 were shown by ESI/MALDI-MS to photogenerate primarily adducts of NADP with deleterious UV and fluorescent properties. Our work stresses the superior
release properties conferred by α-Me substitution on aqueous carboxamide photorelease from o-nitrobenzyl compds.
ACCESSION NUMBER: 2000:380207 CAPLUS
DOCUMENT NUMBER: 133:173856
TITLE: Enzymatic Synthesis of Caged NADP Cofactors: Aqueous NADP Photorelease and Optical Properties
AUTHOR(S): Salerno, Charles P.; Magde, Douglas; Patron, Andrew P.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of California at San Diego, La Jolla, CA, 92093-0506, USA
SOURCE: Journal of Organic Chemistry (2000), 65(13), 3971-3981
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:173856
IT **288591-59-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enzymic synthesis of caged NADP cofactors and aqueous NADP photorelease
and optical properties)
RN 288591-59-3 CAPLUS
CN Benzaldehyde, 4,5-dimethoxy-2-nitro-, O-acetyloxime (9CI) (CA INDEX NAME)



L31 ANSWER 12 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L31 ANSWER 13 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB The second order rate coefficient k2 for elimination reaction of (E)-2,4-(NO2)2C6H4CH:NO2CC6H4X (X = H, p-MeO, m-Br, p-NO2) to 2,4-(NO2)2C6H4CN + XC6H4CO2- promoted by R2NH [Bz(i-Pr)NH, i-Bu2NH, i-Pr2NH, 2,6-DMP] showed excellent correlation with pKa of R2NH on Bronsted plots, with β decreasing as the leaving group is made less basic. Similarly, k2 correlated with the leaving group pKa, with |βlg| decreasing with the stronger base. The results are consistent with an E2 mechanism; the substantial values of β and |βlg| rule out E1cb.
ACCESSION NUMBER: 1999:655305 CAPLUS
DOCUMENT NUMBER: 132:49664
TITLE: Elimination Reactions of (E)-2,4-Dinitrobenzaldehyde O-Benzoyloximes
AUTHOR(S): Cho, Bong Rae; Chung, Hack Sook; Pyun, Sang Yong
CORPORATE SOURCE: Department of Chemistry and Center for Electro- and Photo-Responsive Molecules, Korea University, Seoul, 136-701, S. Korea
SOURCE: Journal of Organic Chemistry (1999), 64(22), 8375-8378
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **252929-76-3P 252929-77-4P 252929-78-5P 252929-79-6P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT
(Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(kinetics, mechanism, and transition state structure for elimination reaction of (E)-2,4-dinitrobenzaldehyde O-benzoyloximes)
RN 252929-76-3 CAPLUS
CN Benzaldehyde, 2,4-dinitro-, O-benzoyloxime, [C(E)]- (9CI) (CA INDEX NAME)

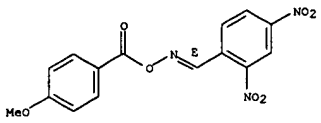
Double bond geometry as shown.



RN 252929-77-4 CAPLUS
CN Benzaldehyde, 2,4-dinitro-, O-(4-methoxybenzoyl)oxime, [C(E)]- (9CI) (CA INDEX NAME)

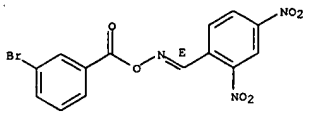
Double bond geometry as shown.

L31 ANSWER 13 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



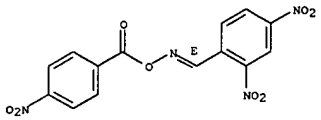
RN 252929-78-5 CAPLUS
CN Benzaldehyde, 2,4-dinitro-, O-(3-bromobenzoyl)oxime, [C(E)]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 252929-79-6 CAPLUS
CN Benzaldehyde, 2,4-dinitro-, O-(4-nitrobenzoyl)oxime, [C(E)]- (9CI) (CA INDEX NAME)

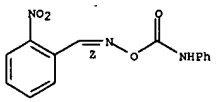
Double bond geometry as shown.



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

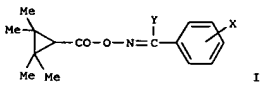
L31 ANSWER 14 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB O-arylcarbamoylated hydroxylamine tosylate reacts with aldehydes at room temperature to give the corresponding O-carbamoylated oximes. The reaction of carbamoylated hydroxylamine with aromatic aldehydes in THF or in toluene at reflux affords the corresponding nitriles and anilinium tosylate in high yield. Attempts to cyclize the O-carbamoylated oximes in the presence of AcCl lead again to the formation of nitriles.
ACCESSION NUMBER: 1999:631975 CAPLUS
DOCUMENT NUMBER: 132:3107
TITLE: Direct conversion of aldehydes to nitriles via O-phenylcarbamoylated aldoximes
AUTHOR(S): Coskun, Necdet; Arikan, Nevin
CORPORATE SOURCE: Department of Chemistry, Uludag University, Bursa, 16059, Turk.
SOURCE: Tetrahedron (1999), 55(40), 11943-11948
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:3107
IT **250722-20-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(direct conversion of aldehydes to nitriles via O-phenylcarbamoylated aldoximes)
RN 250722-20-4 CAPLUS
CN Benzaldehyde, 2-nitro-, O-[(phenylamino)carbonyl]oxime, [C(Z)]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



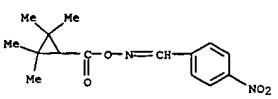
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 15 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
GI



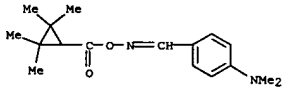
I

AB Twenty new substituted benzaldehyde oxime tetramethylcyclopropane carboxylates I (X = H, 4-C6H5OC6H4, 4-CH3, 4-(CH3)2CH, 4-(CH3)3C, 4-Cl, 4-NO2, 4-NM2, 2-Cl-4-NMe2, 3,5-Cl2NMe2; Y = H, Cl, CN; etc.) were prepared and tested as pesticides. The preliminary bioassays indicated that compds. I (X = 4-Me2N, 4-Et2N; Y = H) showed high insecticidal activity.
ACCESSION NUMBER: 1999:532271 CAPLUS
DOCUMENT NUMBER: 131:286241
TITLE: Synthesis and bioactivity of substituted benzaldehyde oxime carboxylates. (III) - Synthesis and bioactivity of substituted benzaldehyde oxime tetramethylcyclopropanecarboxylates
AUTHOR(S): Ma, Jun-An; Huang, Run-Qiu; Chai, You-Xin
CORPORATE SOURCE: Inst. State Key Elemento-organic Chemistry, Nankai Univ., Tianjin, 300071, Peop. Rep. China
SOURCE: Gaodeng Xuexiao Huaxue Xuebao (1999), 20(5), 747-749
CODEN: KTHPDM; ISSN: 0251-0790
PUBLISHER: Gaodeng Jiaoyu Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
IT **246532-24-1P 246532-31-0P 246532-32-1P 246532-33-2P 246532-34-3P 246532-35-4P 246532-36-5P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of O-tetramethylcyclopropanecarbonyl benzoyloximes as pesticides)
RN 246532-24-1 CAPLUS
CN Benzaldehyde, 4-nitro-, O-[(2,2,3,3-tetramethylcyclopropyl)carbonyl]oxime (9CI) (CA INDEX NAME)

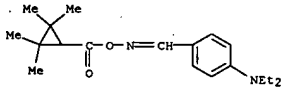


RN 246532-31-0 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[(2,2,3,3-tetramethylcyclopropyl)carbonyl]oxime (9CI) (CA INDEX NAME)

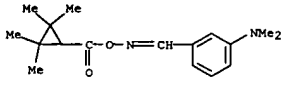
L31 ANSWER 15 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



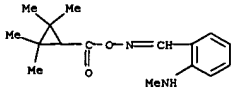
RN 246532-32-1 CAPLUS
CN Benzaldehyde, 4-(diethylamino)-, O-[(2,2,3,3-tetramethylcyclopropyl)carbonyl]oxime (9CI) (CA INDEX NAME)



RN 246532-33-2 CAPLUS
CN Benzaldehyde, 3-(dimethylamino)-, O-[(2,2,3,3-tetramethylcyclopropyl)carbonyl]oxime (9CI) (CA INDEX NAME)

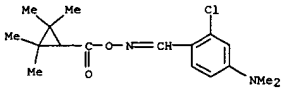


RN 246532-34-3 CAPLUS
CN Benzaldehyde, 2-(methylamino)-, O-[(2,2,3,3-tetramethylcyclopropyl)carbonyl]oxime (9CI) (CA INDEX NAME)

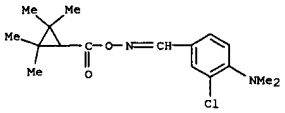


RN 246532-35-4 CAPLUS
CN Benzaldehyde, 2-chloro-4-(dimethylamino)-, O-[(2,2,3,3-tetramethylcyclopropyl)carbonyl]oxime (9CI) (CA INDEX NAME)

L31 ANSWER 15 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 246532-36-5 CAPLUS
CN Benzaldehyde, 3-chloro-4-(dimethylamino)-, O-[(2,2,3,3-tetramethylcyclopropyl)carbonyl]oxime (9CI) (CA INDEX NAME)



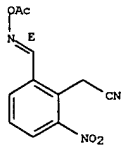
L31 ANSWER 16 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN

AB The N-alkyl- and N-arylisoquinolinium salts reacted with free NH2OH in pyridine to give isoquinoline 2-oxide as final product. The intermediate dioxime 2-HON:CHC6H4CH2CH:NOH (I) was isolated and characterized by derivatization with Ac2O to 2-AcON:CHC6H4CH2CN. From the reaction of I with (CF3CO)2O/Et3N, 3-aminoisoquinoline 2-oxide resulted after hydrolysis. Due to the electronic influence, N-alkylated 5-nitroisoquinolinium salts react faster than the resp. 5-hydroxy derivs., but with the same course of conversion via dioximes to amine oxides. An optimized method for preparation of the amine oxides was developed.

ACCESSION NUMBER: 1999:282639 CAPLUS
DOCUMENT NUMBER: 131:58739
TITLE: Reactions of isoquinolinium salts with hydroxylamine derivatives. 2nd communication. N-Alkyl- and N-aryl-substituted compounds
AUTHOR(S): Mohrle, H.; Niessen, R.
CORPORATE SOURCE: Inst. Pharmazeutische Chem., Heinrich-Heine-Univ., Dusseldorf, D-40225, Germany
SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences (1999), 54(4), 532-540
CODEN: ZNBSEN; ISSN: 0932-0776
PUBLISHER: Verlag der Zeitschrift fuer Naturforschung
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 131:58739

IT **227945-28-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isoquinoline oxides from reaction of isoquinolinium salts with hydroxylamine)
RN 227945-28-0 CAPLUS
CN Benzeneacetonitrile, 2-[(E)-[(acetyloxy)imino]methyl]-6-nitro- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 17 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
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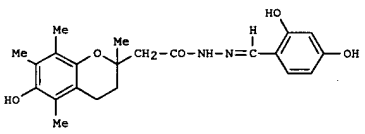


I

AB The title compds. XWY [X = benzene ring, chroman ring, etc.; Y = (un)substituted Ph, etc.; W = CONHN:CH, etc.] are prepared The title compound I in vitro showed IC50 of 4.2 μM against the Maillard reaction.

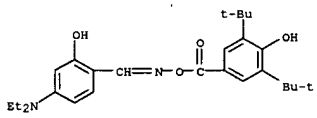
ACCESSION NUMBER: 1999:253739 CAPLUS
DOCUMENT NUMBER: 130:325088
TITLE: Preparation of acylhydrazone derivatives as Maillard reaction inhibitors and active oxygen scavengers
INVENTOR(S): Inoue, Hitoshi; Horigome, Masato; Kinoshita, Nobuhiro; Shibayama, Toshie
PATENT ASSIGNEE(S): Nisshin Flour Milling Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 80 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11106371	A2	19990420	JP 1998-177222	19980624
PRIORITY APPLN. INFO.:			JP 1997-179754 A	19970704

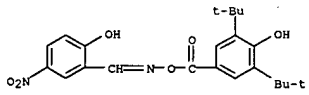
OTHER SOURCE(S): MARPAT 130:325088

IT **223723-34-0P 223723-35-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of acylhydrazone derivs. as Maillard reaction inhibitors and active oxygen scavengers)
RN 223723-34-0 CAPLUS
CN Benzaldehyde, 4-(diethylamino)-2-hydroxy-, O-[3,5-bis(1,1-dimethylethyl)-4-hydroxybenzoyl]oxime (9CI) (CA INDEX NAME)

L31 ANSWER 17 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

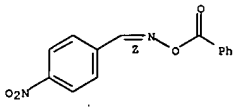


RN 223723-35-1 CAPLUS
CN Benzaldehyde, 2-hydroxy-5-nitro-, O-[3,5-bis(1,1-dimethylethyl)-4-hydroxybenzoyl]oxime (9CI) (CA INDEX NAME)



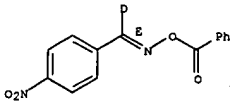
L31 ANSWER 18 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB Elimination reactions of (E)- and (Z)-benzaldehyde O-benzoyloximes 1 and 2
with DBU in MeCN have been investigated kinetically. The reactions are second order and exhibit substantial values of Hammett ρ and kH/kD values, and an E2 mechanism is evident. The rate of elimination from 2 is approx. 36000 fold faster than that from 1. For reactions of 1 with DBU in MeCN, kH/kD = 3.3 ± 0.2, Hammett ρ value of 2.19 ± 0.05, β1g = -0.49 ± 0.02, ΔH.thermod. = 10.4 ± 0.6 kcal/mol, and ΔS.thermod. = -34.3 ± 2.6 eu have been determined The corresponding values for 2 are kH/kD = 7.3 ± 0.2, ρ = 1.21 ± 0.05, β1g = -0.40 ± 0.01, ΔH.thermod. = 6.8 ± 0.5 kcal/mol, and ΔS.thermod. = -25.8 ± 1.9 eu, resp. The results indicate that the anti-eliminations from 2 proceed via more sym. transition states with smaller degrees of proton transfer and Nα-OC(O)Ar bond cleavage, less neg. charge development at the β-carbon, and a greater extent of triple bond formation than that for the syn-elimination.
ACCESSION NUMBER: 1998:446769 CAPLUS
DOCUMENT NUMBER: 129:135759
TITLE: Elimination Reactions of (E)- and (Z)-Benzaldehyde O-Benzoyloximes. Transition State Differences for the Syn- and Anti-Eliminations Forming Nitriles
AUTHOR(S): Cho, Bong Rae; Chung, Hak Suk; Cho, Nam Soon
CORPORATE SOURCE: Department of Chemistry, Korea University, Seoul, 136-701, S. Korea
SOURCE: Journal of Organic Chemistry (1998), 63(14), 4685-4690
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **18322-89-9P 210645-51-5P 210645-52-6P 210645-53-7P 210645-54-8P 210645-65-1P 210645-66-2P 210645-67-3P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(syn- and anti-elimination transition state differences for nitrile formation from (E)- and (Z)-benzaldehyde O-benzoyloximes)
RN 18322-89-9 CAPLUS
CN Benzaldehyde, 4-nitro-, O-benzoyloxime, [C(Z)]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



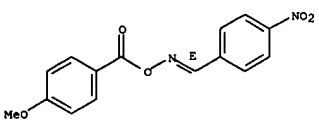
RN 210645-51-5 CAPLUS
CN Benzaldehyde-formyl-d, 4-nitro-, O-benzoyloxime, [C(E)]- (9CI) (CA INDEX NAME)

L31 ANSWER 18 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
Double bond geometry as shown.



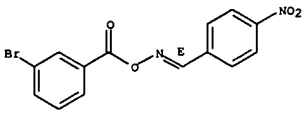
RN 210645-52-6 CAPLUS
CN Benzaldehyde, 4-nitro-, O-(4-methoxybenzoyl)oxime, [C(E)]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



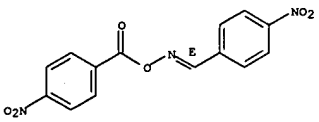
RN 210645-53-7 CAPLUS
CN Benzaldehyde, 4-nitro-, O-(3-bromobenzoyl)oxime, [C(E)]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



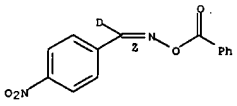
RN 210645-54-8 CAPLUS
CN Benzaldehyde, 4-nitro-, O-(4-nitrobenzoyl)oxime, [C(E)]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



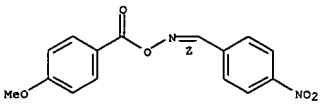
L31 ANSWER 18 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 210645-65-1 CAPLUS
CN Benzaldehyde-formyl-d, 4-nitro-, O-benzoyloxime, [C(Z)]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



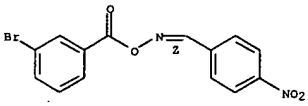
RN 210645-66-2 CAPLUS
CN Benzaldehyde, 4-nitro-, O-(4-methoxybenzoyl)oxime, [C(Z)]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 210645-67-3 CAPLUS
CN Benzaldehyde, 4-nitro-, O-(3-bromobenzoyl)oxime, [C(Z)]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 19 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
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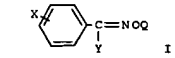
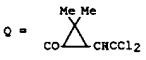
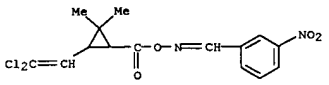


I

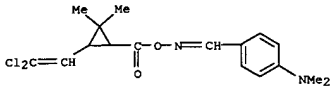


AB Twenty title pyrethroid oxime-esters I (X = 4-tert-Bu, 3,4-OCH2O, 2,4-Cl2, 3-NO2, 4-NMe2; Y = H, NMe2, NHEt, N(CH2)5, 1,2,4-triazol-1-yl, cyclohexylamino, C6H5NH, NH2, NEt2; Q as shown) were prepared from t-BuOCl chloronation of I (Q = H; X = above) followed by condensation with QCl in the presence of Et3N. The bioassay indicated that compds. I (X = 4-tert-Bu, 4-NMe2; Y = H; Q as shown) showed antiviral activities and I (X = 4-Cl; Y = H; Q as shown) showed antibacterial activity.
ACCESSION NUMBER: 1998:207620 CAPLUS
DOCUMENT NUMBER: 128:294898
TITLE: Synthesis and bioactivity of substituted benzaldoxime carboxylate. I. Synthesis and bioactivity of substituted benzaldoxime 3-(2,2-dichloroethenyl)-2,2-dimethyl cyclopropanecarboxylates
AUTHOR(S): Huang, Runqiu; Sun, Jianyu; Ma, Jun'an; Li, Huiying
CORPORATE SOURCE: Inst. Elemento-Organic Chem., Nankai Univ., Tianjin, 300071, Peop. Rep. China
SOURCE: Yingyong Huaxue (1998), 15(1), 9-12
CODEN: YIHUED; ISSN: 1000-0518
PUBLISHER: Yingyong Huaxue Bianji Weiyuanhui
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
IT **205937-81-1P 205937-83-3P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and bioactivity of substituted benzaldoxime carboxylate derivs.)
RN 205937-81-1 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[[3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropyl]carbonyl]oxime (9CI) (CA INDEX NAME)

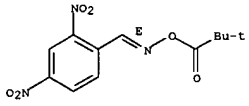
L31 ANSWER 19 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 205937-83-3 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[[3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropyl]carbonyl]oxime (9CI) (CA INDEX NAME)



L31 ANSWER 20 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 20 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN

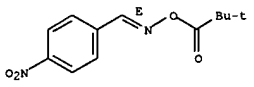
AB Elimination reactions of (E)-2,4-dinitrobenzaldehyde O-pivaloyloxime promoted by R2NH/R2NH2+ buffer in 70% MeCN(aq) have been studied kinetically. The reaction exhibited second order kinetics and general base catalysis with Bronsted β=0.45. The Hammett ρ value decreased from 2.3 to 1.6 as the base-solvent system was changed from DBU in MeCN to R2NH/R2NH2+ buffer in 70% MeCN(aq). From these results an E2 mechanism is proposed.

ACCESSION NUMBER: 1998:47440 CAPLUS
DOCUMENT NUMBER: 128:167060
TITLE: Mechanism of elimination from (E)-2,4-dinitrobenzaldehyde O-pivaloyloxime promoted by R2NH/R2NH2+ buffer in 70% MeCN (aq)
AUTHOR(S): Cho, Bong Rae; Cho, Nam Soon; Chung, Hak Suk; Son, Ki Nam; Han, Man So; Pyun, Sang Yong
CORPORATE SOURCE: Department of Chemistry, Korea University, Seoul, 136-701, S. Korea
SOURCE: Bulletin of the Korean Chemical Society (1997), 18(12), 1301-1304
CODEN: BKCSDE; ISSN: 0253-2964
PUBLISHER: Korean Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **149540-92-1**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT
(Reactant); PROC (Process); RACT (Reactant or reagent)
(mechanism of elimination from (E)-2,4-dinitrobenzaldehyde O-pivaloyloxime promoted by R2NH/R2NH2+ buffer in 70% MeCN (aq))

RN 149540-92-1 CAPLUS
CN Benzaldehyde, 4-nitro-, O-(2,2-dimethyl-1-oxopropyl)oxime, [C(E)]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

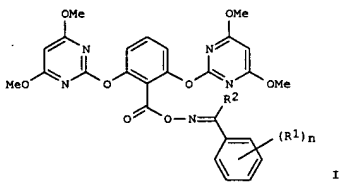


IT **203127-48-4P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT
(Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(mechanism of elimination from (E)-2,4-dinitrobenzaldehyde O-pivaloyloxime promoted by R2NH/R2NH2+ buffer in 70% MeCN (aq))

RN 203127-48-4 CAPLUS
CN Benzaldehyde, 2,4-dinitro-, O-(2,2-dimethyl-1-oxopropyl)oxime, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L31 ANSWER 21 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
GI



I

AB The title compds. I [R1 represents hydrogen, halogen, cyano, nitro, alkyl,
cycloalkyl, alkoxy, alkenyloxy, alkylthio, amino which can be substituted with alkyl, aryl, aryloxy, acyl or acyloxy; n denotes an integer of 1 to 5; and R2 represents hydrogen, halogen, cyano, nitro, alkyl, alkoxy, alkylthio, alkoxycarbonyl, alkenyloxycarbonyl, arylmethoxycarbonyl, heteroarylmethoxy carbonyl, alkylaminocarbonyl, di(alkyl)aminocarbonyl, arylmethylaminocarbonyl, heteroarylmethylaminocarbonyl, or Ph which can be
substituted with R1] are prepared by reacting 2-(4,6-dimethoxypyrimidin-2-yl)oxy-6-hydroxybenzoic acid oxime ester derivs. with appropriate pyrimidine derivs., e.g., 4,6-dimethoxy-2-alkylsulfonylpyrimidine. Thus, a mixture of 2-(4,6-dimethoxypyrimidin-2-yl)oxy-6-hydroxybenzoic acid benzophenone oxime ester, potassium carbonate, and 4,6-dimethoxy-2-methylsulfonylpyrimidine in DMF was stirred at 80° to give, after workup, 2,6-di(4,6-dimethoxypyrimidin-2-yl)oxybenzoic acid benzophenone oxime ester.

ACCESSION NUMBER: 1997:734617 CAPLUS
DOCUMENT NUMBER: 127:318973
TITLE: Process for preparing 2,6-di(4,6-dimethoxypyrimidin-2-yl)oxybenzoic acid oxime ester derivatives as herbicides
INVENTOR(S): Kim, Kun-Tai; Lee, Byoung-Bae; Joe, Goon-Ho; Ahn, Sei-Chang; Kang, Chang-Mo; Lee, Seong-Min; Bae, Jae-Soon; Cho, Jin-Ho; Lee, Sang-Ho; Choi, Nak-Hee; Sa, Jong-Sin
PATENT ASSIGNEE(S): Lg Chemical Ltd., S. Korea
SOURCE: Can. Pat. Appl., 65 pp.
CODEN: CPXXEB
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

L31 ANSWER 21 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

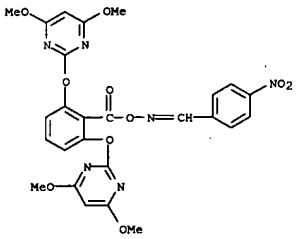
CA 2194080	AA	19970629	CA 1996-2194080		19961227
CA 2194080	C	20000418			
KR 209293	B1	19990715	KR 1996-2737		19960205
KR 212636	B1	19990802	KR 1996-61015		19961202
PRIORITY APPLN. INFO.:			KR 1995-61160	A	19951228
			KR 1996-2737	A	19960205
			KR 1996-43480	A	19961001

OTHER SOURCE(S): CASREACT 127:318973; MARPAT 127:318973

IT **168088-55-9P**
RL: AGR (Agricultural use); IMF (Industrial manufacture); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(process for preparing herbicidal di[(dimethoxypyrimidinyl)oxy]benzoic acid oxime ester derivs.)

RN 168088-55-9 CAPLUS

CN Benzaldehyde, 4-nitro-, O-[2,6-bis[(4,6-dimethoxy-2-pyrimidinyl)oxy]benzoyl]oxime (9CI) (CA INDEX NAME)



L31 ANSWER 22 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN

AB Elimination reactions of (E)- and (Z)-benzaldehyde O-pivaloyloximes 1 and 2 with DBU in MeCN have been investigated kinetically. The reactions are second order and exhibit substantial values of Hammett ρ and kH/kD values, and an E2 mechanism is evident. The rate of elimination from 2 is approx. 20 000-fold faster than that from 1. For reactions of 1 with DBU in MeCN, a Hammett ρ values of 2.4 ± 0.1, kH/kD = 2.7 ± 0.3, ΔH.thermod. = 12.5 ± 0.2 kcal/mol, and ΔS.thermod. = -31.0 ± 0.6 eu have been determined The corresponding values for 2 are ρ = 1.4 ± 0.1, kH/kD = 7.8 ± 0.3, ΔH.thermod. = 8.8 ± 0.1 kcal/mol, and ΔS.thermod. = -23.6 ± 0.4 eu, resp. The results indicate that the nitrile-forming anti eliminations from 2 proceed via a more sym. transition state with a smaller degree of proton transfer, less neg. charge development at the β-carbon, and greater extent of triple-bond formation than that for the syn elimination.

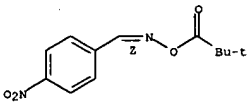
ACCESSION NUMBER: 1997:231039 CAPLUS
DOCUMENT NUMBER: 126:263711
TITLE: Elimination Reactions of (E)- and (Z)-Benzaldehyde O-Pivaloyloximes. Transition-State Differences for the Syn and Anti Eliminations Forming Nitriles
AUTHOR(S): Cho, Bong Rae; Cho, Nam Soon; Lee, Sang Kook
CORPORATE SOURCE: Department of Chemistry, Korea University, Seoul, 136-701, S. Korea
SOURCE: Journal of Organic Chemistry (1997), 62(7), 2230-2233
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **188799-40-8P**
RL: PEP (Physical, engineering or chemical process); PNU (Preparation, unclassified); PRP (Properties); RCT (Reactant); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(transition-state differences for syn and anti eliminations forming nitriles from (E)- and (Z)-benzaldehyde O-pivaloyloximes)

RN 188799-40-8 CAPLUS

CN Benzaldehyde, 4-nitro-, O-(2,2-dimethyl-1-oxopropyl)oxime, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



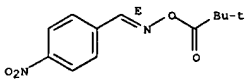
IT **149540-92-1**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(transition-state differences for syn and anti eliminations forming nitriles from (E)- and (Z)-benzaldehyde O-pivaloyloximes)

RN 149540-92-1 CAPLUS

CN Benzaldehyde, 4-nitro-, O-(2,2-dimethyl-1-oxopropyl)oxime, [C(E)]- (9CI)

L31 ANSWER 22 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
(CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 23 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN

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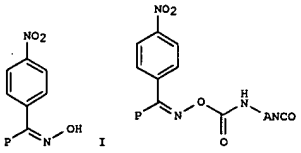
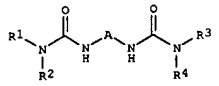


I

II



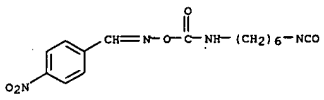
III

AB A general method for preparation of bis[ureas] was developed from oxime resin-derived carbamates of diisocyanates. Thus, monoaddn. of diisocyanates a polymer-supported 4-nitrobenzaldehyde oxime I (P = polymer support) gave isocyanates II (P = polymer support; A = alkanediyl). Treatment of II with amines gave the alkanediylbis[ureas] III (R1-R4 = alkyl, cyclohexylmethyl, 4-morpholinyl, etc.). Directional urea synthesis was achieved by sequential amine addition which demonstrated the utility of thermolabile oxime-derived carbamate linkages to a polymer support. The products, obtained in good yield in three steps, were of high chemical purity.

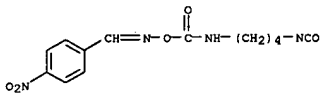
ACCESSION NUMBER: 1996:683459 CAPLUS
DOCUMENT NUMBER: 126:74337
TITLE: Diisocyanates as scaffolds for combinatorial libraries. The solid-phase synthesis of bis[ureas] from polymer-supported diisocyanates
AUTHOR(S): Scialdone, Mark A.
CORPORATE SOURCE: DuPont Central Res. and Development, Wilmington, DE, 19880-0328, USA
SOURCE: Tetrahedron Letters (1996), 37(45), 8141-8144
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **185432-96-6DP**, polymer-supported **185432-97-7DP**, polymer-supported **185432-98-8DP**, polymer-supported **185432-99-9DP**, polymer-supported **185433-00-5DP**, polymer-supported **185433-01-6DP**, polymer-supported
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of alkanediylbis[ureas] from polymer-supported diisocyanates)

L31 ANSWER 23 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 185432-96-6 CAPLUS
CN Benzaldehyde, 4-nitro-, O-[[(6-isocyanatohexyl)amino]carbonyl]oxime (9CI) (CA INDEX NAME)

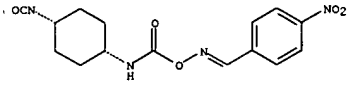


RN 185432-97-7 CAPLUS
CN Benzaldehyde, 4-nitro-, O-[[(4-isocyanatobutyl)amino]carbonyl]oxime (9CI) (CA INDEX NAME)

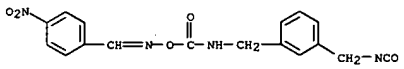


RN 185432-98-8 CAPLUS
CN Benzaldehyde, 4-nitro-, O-[[(4-isocyanatocyclohexyl)amino]carbonyl]oxime, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



RN 185432-99-9 CAPLUS
CN Benzaldehyde, 4-nitro-, O-[[[[3-(isocyanatomethyl)phenyl]methyl]amino]carbonyl]oxime (9CI) (CA INDEX NAME)



RN 185433-00-5 CAPLUS
CN Benzaldehyde, 4-nitro-, O-[[[1-[3-(1-isocyanato-1-methylethyl)phenyl]-1-methylethyl]amino]carbonyl]oxime (9CI) (CA INDEX NAME)

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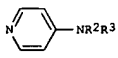
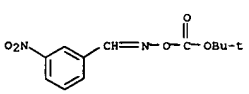


IV

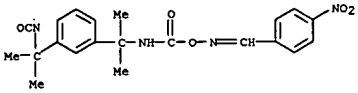
AB R1CH:NOC(O)OR4 [I; R1 = acyl, (substituted) hydrocarbyl, (substituted) heterocyclyl; R4 = alkyl, alkenyl, aralkyl] are prepared by reaction of R1CH:NOH (II; R1 = same as I) with R4OC(O)OC(O)OR4 (III; R4 = same as I) in presence of 0.01-5 mol.% (based on II) aminopyridines IV (R2, R3 = alkyl, aryl; R2R3 may form ring). II (R1 = Ph) was treated with III (R4 = CMe3) and IV (R2 = R3 = Me) in CH2Cl2 at 20° for 8 h to give 97.7% I (R1 = Ph, R4 = CMe3).
ACCESSION NUMBER: 1996:523557 CAPLUS
DOCUMENT NUMBER: 125:167339
TITLE: Preparation of aldoxime carbonates
INVENTOR(S): Iwasaki, Fumiaki; Mitsuharu, Michiko
PATENT ASSIGNEE(S): Tokuyama Corp, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08151357	A2	19960611	JP 1994-291593	19941125
JP 3295258	B2	20020624		
PRIORITY APPLN. INFO.:			JP 1994-291593	19941125

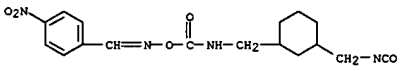
OTHER SOURCE(S): CASREACT 125:167339; MARPAT 125:167339
IT **180308-36-5P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of aldoxime carbonates from aldoximes and dicarbonates with aminopyridine catalysts)
RN 180308-36-5 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[(1,1-dimethylethoxy)carbonyl]oxime (9CI) (CA INDEX NAME)



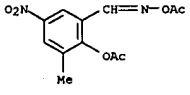
L31 ANSWER 23 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 185433-01-6 CAPLUS
CN Benzaldehyde, 4-nitro-, O-[[[[3-(isocyanatomethyl)cyclohexyl]methyl]amino]carbonyl]oxime (9CI) (CA INDEX NAME)



L31 ANSWER 25 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB Optically active salicyloxazolines were obtained by condensation of salicylcarboximidates with chiral aminoalcs. In the enantioselective copper-catalyzed cyclopropanation of styrene with Et diazoacetate optical inductions up to 60% ee were achieved with these ligands. An example ligand is (4S-cis)-4,5-dihydro-2-(2-hydroxyphenyl)-5-phenyl-4-oxazolemethanol. Low asym. induction was obtained with 2-[[[1-(hydroxymethyl)propyl]imino]methyl]phenol as ligand.
ACCESSION NUMBER: 1995:847417 CAPLUS
DOCUMENT NUMBER: 124:86845
TITLE: Enantioselective catalysis. 971. Optically active salicyloxazoline ligands in enantioselective copper-catalyzed cyclopropanation reactions
AUTHOR(S): Brunner, Henri; Berghofer, Josef
CORPORATE SOURCE: Institut fuer Anorganische Chemie, Universitaet Regensburg, Universitaetsstrasse 31, Regensburg, 93053, Germany
SOURCE: Journal of Organometallic Chemistry (1995), 501(1-2), 161-6
CODEN: JORCAI; ISSN: 0022-328X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:86845
IT **172532-29-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(chiral (hydroxyphenyl)oxazolemethanols as ligands for copper-catalyzed cyclopropanation)
RN 172532-29-5 CAPLUS
CN Benzaldehyde, 2-(acetyloxy)-3-methyl-5-nitro-, 1-(O-acetyloxime) (9CI) (CA INDEX NAME)



L31 ANSWER 26 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
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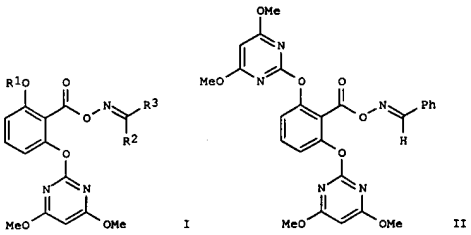


AB The invention relates to novel herbicidal pyrimidine derivs. I [R1 = 4,6-dimethoxy-2-pyrimidinyl, C1-4 alkyl, C2-4 alkenyl, acyl, alkylsulfonyl or heteroarylmethyl; R2 = H, halo, cyano, NO2, C1-8 alkyl, C1-8 alkoxy, C1-8 alkythio, C1-8 alkoxycarbonyl, C2-4 alkenyloxycarbonyl, (hetero)arylmethoxycarbonyl, C1-4 alkylaminocarbonyl, aryl-C1-4 alkylaminocarbonyl, heteroarylmethylaminocarbonyl, aryl, C2-8 alkenyl, C3-6 cycloalkyl, PhCH2, aryloxy, arylthio, or C1-8 alkylcarbonyl; R3 = (un)substituted Ph, COR4; R4 = H, C1-4 alkyl, C2-4 alkenyl, C3-6 cycloalkyl, PhCH2, aryl, C1-4 alkoxy, C2-4 alkenyloxy, C3-6 cycloalkoxy, PhCH2O, aryloxy, C1-4 alkythio, C2-4 alkenylthio, C3-6 cycloalkylthio, PhCH2S, arythio, amino which can be substituted with C1-C4 alkyl or aryl or arylmethyl], as well as a process for their preparation, and their herbicidal compns. I have excellent activity against both narrow- and broadleaf weeds, with increased safety for crops (especially directly sown rice). For example, 2,6-bis(4,6-dimethoxypyrimidin-2-yl)oxybenzoic acid was treated with 2,2'-dipyridyl disulfide and PPh3 in PhMe to give 90% of the corresponding 2-pyridyl thioester, which reacted with benzaldehyde oxime in CH2Cl2 in the presence of CuBr2 to give 85% title compound II. At 63 g/ha postemergence under paddy field conditions, II gave complete control of 7 weeds with no damage to direct-sown rice seedlings. Characterizing phys. and herbicidal data for 73 compds. are given.

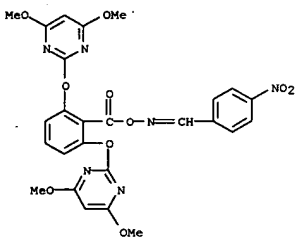
ACCESSION NUMBER: 1995:810566 CAPLUS
DOCUMENT NUMBER: 123:228208
TITLE: Pyrimidine derivatives, process for their preparation, and their use as herbicides.
INVENTOR(S): Hur, Chang Uk; Cho, Jin Ho; Hong, Su Myeong; Kim, Hong Woo; Lim, Young Hee; Rim, Jae Suk; Kim, Jeong Su; Chae, Sang Heon
PATENT ASSIGNEE(S): Lucky Ltd., S. Korea
SOURCE: Eur. Pat. Appl., 54 pp.

L31 ANSWER 26 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 658549	A1	19950621	EP 1994-117857	19941111
EP 658549	B1	20010523		
R: CH, DE, FR, GB, LI, NL				
KR 9701480	B1	19970206	KR 1993-24099	19931113
KR 120271	B1	19971104	KR 1993-30055	19931227
KR 120270	B1	19971104	KR 1993-31016	19931229
US 5521146	A	19960528	US 1994-339249	19941110
BR 9404436	A	19951017	BR 1994-4436	19941111
CN 1111623	A	19951115	CN 1994-117926	19941111
CN 1043885	B	19990630		
AU 9478812	A1	19950608	AU 1994-78812	19941114
AU 673629	B2	19961114		
JP 07196629	A2	19950801	JP 1994-279506	19941114
JP 2517215	B2	19960724		

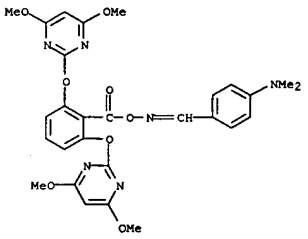
PRIORITY APPLN. INFO.: KR 1993-24099 A 19931113
KR 1993-30055 A 19931227
KR 1993-31016 A 19931229

OTHER SOURCE(S): CASREACT 123:228208; MARPAT 123:228208
IT **168088-55-9P 168088-63-9P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidine derivs. as herbicides)
RN 168088-55-9 CAPLUS
CN Benzaldehyde, 4-nitro-, O-[2,6-bis[(4,6-dimethoxy-2-pyrimidinyl)oxy]benzoyl]oxime (9CI) (CA INDEX NAME)



RN 168088-63-9 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[2,6-bis[(4,6-dimethoxy-2-

L31 ANSWER 26 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
pyrimidinyl)oxy]benzoyl]oxime (9CI) (CA INDEX NAME)



L31 ANSWER 27 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
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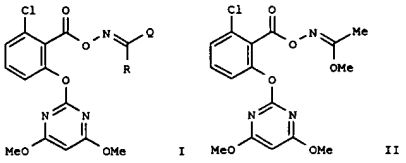


AB New 6-chloro-2-[(4,6-dimethoxy-2-pyrimidinyl)oxy]benzoates [[2-[[(alkyleneamino)oxy]carbonyl]-1-chloro-3-phenoxy]pyrimidines] I (R = H, halo, cyano, etc.; Q = alkyl, alkenyl, cycloalkyl, etc.) were disclosed. I were claimed as herbicides. An example compound 2-[1-chloro-[[[(1-methoxyethylidene)amino]oxy]carbonyl]phenoxy]-4,6-dimethoxypyrimidine (II) was prepared

ACCESSION NUMBER: 1994:605344 CAPLUS
DOCUMENT NUMBER: 121:205344
TITLE: Novel 6-chloro-2-(4,6-dimethoxypyrimidin-2-yl) oxybenzoic acid ester derivatives, processes for their production and their application as herbicides.
INVENTOR(S): Hur, Chang Uk; Cho, Jin Ho; Lee, Ho Seong; Yoo, Sang Ku; Hong, Su Myeong; Kim, Hong Woo; Rim, Jae Suk; Bae, Yeong Tae; Chae, Sand Heon; et al.
PATENT ASSIGNEE(S): Lucky Ltd., S. Korea
SOURCE: Eur. Pat. Appl., 82 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 608862	A1	19940803	EP 1994-101132	19940126
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
KR 9603323	B1	19960308	KR 1993-1017	19930127
KR 9612180	B1	19960916	KR 1993-10097	19930604
KR 9612179	B1	19960916	KR 1993-10098	19930604
KR 9612181	B1	19960916	KR 1993-10099	19930604
KR 9612194	B1	19960916	KR 1993-10100	19930604
KR 9612195	B1	19960916	KR 1993-10101	19930604
CN 1101345	A	19950412	CN 1994-102665	19940126
US 5494888	A	19960227	US 1994-186589	19940126
BR 9400365	A	19940816	BR 1994-365	19940127
JP 07149735	A2	19950613	JP 1994-7824	19940127
JP 2543665	B2	19961016		

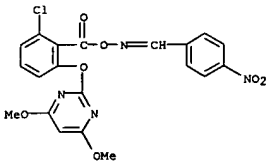
L31 ANSWER 27 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

IN 182571	A	19990508	IN 1994-DE86		19940128
IN 183197	A	19991002	IN 1994-DE1445		19941111
PRIORITY APPLN. INFO.:			KR 1993-1017	A	19930127
			KR 1993-10097	A	19930604
			KR 1993-10098	A	19930604
			KR 1993-10099	A	19930604
			KR 1993-10100	A	19930604
			KR 1993-10101	A	19930604
			EP 1994-101132	A	19940126

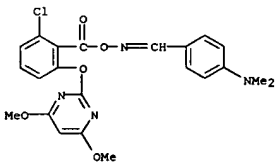
OTHER SOURCE(S): MARPAT 121:205344

IT **157990-17-5P 157990-18-6P 157990-32-4P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide)

RN 157990-17-5 CAPLUS
CN Benzaldehyde, 4-nitro-, O-[2-chloro-6-[(4,6-dimethoxy-2-pyrimidinyl)oxy]benzoyl]oxime (9CI) (CA INDEX NAME)

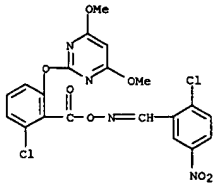


RN 157990-18-6 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[2-chloro-6-[(4,6-dimethoxy-2-pyrimidinyl)oxy]benzoyl]oxime (9CI) (CA INDEX NAME)



RN 157990-32-4 CAPLUS

L31 ANSWER 27 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN Benzaldehyde, 2-chloro-5-nitro-, O-[2-chloro-6-[(4,6-dimethoxy-2-pyrimidinyl)oxy]benzoyl]oxime (9CI) (CA INDEX NAME)



L31 ANSWER 28 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN

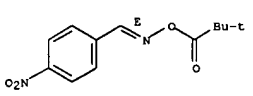
AB Elimination reactions of (E)-O-pivaloylbenzaldoximes promoted by Et3N-MeCN, tert-BuOK-tert-BuOH, and tert-BuOK-DMSO have been studied kinetically. The reactions produce benzonitrile quant. The reactions are second-order and exhibit substantial values of α, β, and kH/kD, and an E2 mechanism is evident. The relative rates of elimination from (E)-O-pivaloylbenzaldoxime were 1, 14.8, and 4.31 + 104 for the above systems, resp. The kH/kD value increased, but the Hammett ρ value increased and then decreased, with this change in the base-solvent system. These results are compared with the predictions of the More O'Ferrall-Jencks reaction coordinate diagram to assess its scope and limitations in the interpretation of the elimination reactions.

ACCESSION NUMBER:	1993:516591 CAPLUS
DOCUMENT NUMBER:	119:116591
TITLE:	Elimination reactions of (E)-O-pivaloylbenzaldoximes
AUTHOR(S):	Cho, Bong Rae; Jang, Wan Jin; Je, Jong Tae; Bartsch, Richard A.
CORPORATE SOURCE:	Dep. Chem., Korea Univ., Seoul, S. Korea
SOURCE:	Journal of Organic Chemistry (1993), 58(15), 3901-4 CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE:	Journal
LANGUAGE:	English

IT **149540-92-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(elimination reaction of, kinetics of)

RN 149540-92-1 CAPLUS
CN Benzaldehyde, 4-nitro-, O-(2,2-dimethyl-1-oxopropyl)oxime, [C(E)]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



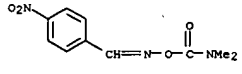
L31 ANSWER 29 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN

AB Thermal decomposition of syn-RCH:NOCONMe2 [I: R = 2-pyridyl, 4-C6H4NO2, Ph, 4-C6H4NMe2, 2,4- or 2,5-C6H3(OMe)2, 2-methyl- or 2-methoxy-4-dimethylaminophenyl, 2-methoxy-1-naphthyl] and syn-RCH:NOBz [II: R = Ph, 4-C6H4OMe, 2,4-C6H3(OMe)2, 2- or 4-methoxy-1-naphthyl, 1,5-C10H6SO2NEt2, 2-benzyloxy-1-naphthyl] at 80-130° was kinetically studied. The decomposition was 1st-order for both I and II, and electron donating groups and substituents at the ortho position increased the reaction rates. Activation entropy values for I and II were very different and, hence, different decomposition mechanisms were proposed: β-elimination with syn/anti isomerization for I and concerted elimination via a cyclic 6-membered ring transition for II.

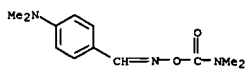
ACCESSION NUMBER:	1992:469340 CAPLUS
DOCUMENT NUMBER:	117:69340
TITLE:	Reaction control of thermal decomposition of aromatic aldoxime derivatives as heat decomposing precursor compounds
AUTHOR(S):	Kawata, Ken; Kitaguchi, Hiroshi; Sato, Kozo; Yabuki, Yoshiharu
CORPORATE SOURCE:	Ashigara Res. Lab., Fuji Photo Film Co., Ltd., Kanagawa, 250-01, Japan
SOURCE:	Senryo to Yakuhin (1992), 37(2), 33-40 CODEN: SETYAL; ISSN: 0370-9671
DOCUMENT TYPE:	Journal
LANGUAGE:	Japanese

IT **93369-36-9 93369-38-1 95186-87-1 142554-04-9**
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(thermal decomposition of, kinetics of, substituent effect and mechanism in relation to)

RN 93369-36-9 CAPLUS
CN Benzaldehyde, 4-nitro-, O-[(dimethylamino)carbonyl]oxime (9CI) (CA INDEX NAME)

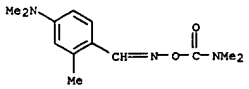


RN 93369-38-1 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[(dimethylamino)carbonyl]oxime (9CI) (CA INDEX NAME)

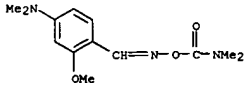


RN 95186-87-1 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-2-methyl-, O-[(dimethylamino)carbonyl]oxim

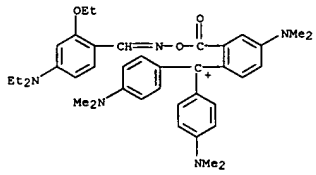
L31 ANSWER 29 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
e (9CI) (CA INDEX NAME)



RN 142554-04-9 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-2-methoxy-, O-[(dimethylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



L31 ANSWER 30 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



CM 2

CRN 14874-70-5
CMF B F4
CCI CCS

L31 ANSWER 30 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
GI For diagram(s), see printed CA Issue.
AB The title materials contain a thermally decolorizable dye I or II [R, R1 =
aryl, heteroaryl, R and R1 may form a ring; R2 = alkyl, alkenyl, aralkyl, aryl, heteroaryl; A = 5- or 6-membered ring; (all the groups, rings, and the benzoquinone ring of II may be substituted; X- = monovalent anion). The materials provide decolored images on heating. Thus, a poly(ethylene terephthalate) film was coated with a heat-sensitive layer containing III to
give a blue thermal recording film.
ACCESSION NUMBER: 1991:52979 CAPLUS
DOCUMENT NUMBER: 114:52979
TITLE: Recording materials using thermally decolorizable dyes
INVENTOR(S): Sato, Kozo
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

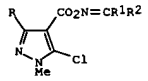
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02164590	A2	19900625	JP 1988-320164	19881219
JP 07084104	B4	19950913		
US 4981833	A	19910101	US 1989-452650	19891219
PRIORITY APPLN. INFO.:			JP 1988-320164 A	19881219

IT **131420-03-6P**
RL: PREP (Preparation)
(preparation of, thermally decolorizable dye, thermal recording material
using)
RN 131420-03-6 CAPLUS
CN Methylium, [2-[[[[4-(diethylamino)-2-ethoxyphenyl]methylene]amino]oxy]carbonyl]-4-(dimethylamino)phenyl]bis[4-(dimethylamino)phenyl]-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 131420-02-5
CMF C39 H48 N5 O3

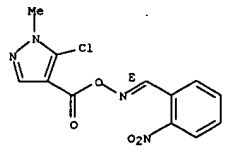
L31 ANSWER 31 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
GI



I

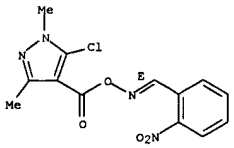
AB A series of novel 1,3-substituted 5-chloropyrazole-4-carboxylic acid oxime
esters I (R = H, Me; R1 = H, Me, Et; R2 = Ph, Me, substituted Ph; R1R2 = cyclohexylidene) was synthesized. Their chemical structures were elucidated
by 1H, 13C-NMR and IR spectra. Fifteen such compds. were screened for their antifungal activity. The results showed that pyrazole oxime esters with electron withdrawing groups had better biol. activities than those with electron releasing groups.
ACCESSION NUMBER: 1991:23855 CAPLUS
DOCUMENT NUMBER: 114:23855
TITLE: Synthesis and antifungal activity of 1,3-substituted 5-chloropyrazole-4-carboxylic acid oxime esters
AUTHOR(S): Khim, Yong Whan; Park, Chi Hyun; Choi, Weon Seok; Kwon, Young Chil; Park, Chang Kyu
CORPORATE SOURCE: OCI Res. Cent., Inchon, S. Korea
SOURCE: Han'guk Nonghwa Hakhoechi (1989), 32(4), 401-7
CODEN: JKACA7; ISSN: 0368-2897
DOCUMENT TYPE: Journal
LANGUAGE: Korean
IT **131141-96-3P 131142-06-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and fungicidal activity of)
RN 131141-96-3 CAPLUS
CN Benzaldehyde, 2-nitro-, O-[(5-chloro-1-methyl-1H-pyrazol-4-yl)carbonyl]oxime, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 131142-06-8 CAPLUS
CN Benzaldehyde, 2-nitro-, O-[(5-chloro-1,3-dimethyl-1H-pyrazol-4-yl)carbonyl]oxime, (E)- (9CI) (CA INDEX NAME)

L31 ANSWER 31 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
Double bond geometry as shown.



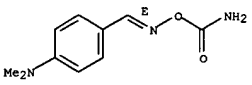
L31 ANSWER 32 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB The 1H and 13C NMR spectra were assigned for a series of O-carbamoyloximes of ortho- and para-substituted benzaldehyde. These compds. exist exclusively in the E configuration. The aromatic protons and carbons show correlations with the appropriate substituent-induced shifts and with Hammett parameters.

ACCESSION NUMBER: 1990:405571 CAPLUS
DOCUMENT NUMBER: 113:5571
TITLE: Proton and carbon-13 NMR studies of some O-carbamoyloximes
AUTHOR(S): Wazeer, Mohammed I. M.; Ali, S. A.; Arab, Mohammed
CORPORATE SOURCE: Chem. Dep., King Fahd Univ. Pet. Miner., Dhahran, 31261, Saudi Arabia
SOURCE: Magnetic Resonance in Chemistry (1989), 27(11), 1102-4
CODEN: MRCHEG; ISSN: 0749-1581
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **127479-16-7 127479-17-8**
RL: PRP (Properties)
(proton and carbon-13 NMR of)

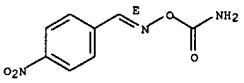
RN 127479-16-7 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(aminocarbonyl)oxime, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 127479-17-8 CAPLUS
CN Benzaldehyde, 4-nitro-, O-(aminocarbonyl)oxime, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



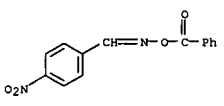
L31 ANSWER 33 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB A photothermog. material has ≥1 shielding layers which temporarily shield acid activity. The shielding layers may contain a fusible agent or a substance which is dissolved in or expanded with the fusible agent under heat-developing temperature The photothermog. material shows improved heat-developing stability and storage stability:

ACCESSION NUMBER: 1988:501932 CAPLUS
DOCUMENT NUMBER: 109:101932
TITLE: Photothermographic material with improved heat-developing stability and storage stability
INVENTOR(S): Goto, Sohei; Komamura, Tawara; Kono, Junichi
PATENT ASSIGNEE(S): Konica Co., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 45 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

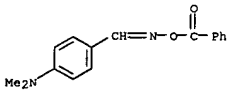
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63004233	A2	19880109	JP 1986-147284	19860624
JP 08012412	B4	19960207		
PRIORITY APPLN. INFO.:			JP 1986-147284	19860624

IT **3848-35-9 4058-69-9**
RL: USES (Uses)
(acid precursor, fusible agent containing, for photothermog. material)

RN 3848-35-9 CAPLUS
CN Benzaldehyde, 4-nitro-, O-benzoyloxime (9CI) (CA INDEX NAME)



RN 4058-69-9 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-benzoyloxime (9CI) (CA INDEX NAME)



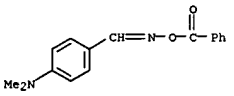
L31 ANSWER 34 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB A photothermog. material comprising a support, photosensitive Ag halide, color-formers, a reducing agent, a binder, and microcapsules is claimed wherein the microcapsule core material contains an acid and/or an acid-precursor. The material retains high contrast even after prolonged storage.

ACCESSION NUMBER: 1988:430203 CAPLUS
DOCUMENT NUMBER: 109:30203
TITLE: Photothermographic material containing microencapsulated acid(-precursor) for improved storage stability
INVENTOR(S): Okauchi, Ken; Kakuchi, Hiroyuki; Yamazaki, Hiroshi
PATENT ASSIGNEE(S): Konica Co., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 45 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

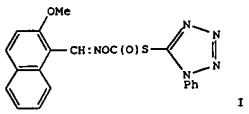
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62288837	A2	19871215	JP 1986-132473	19860607
JP 05079977	B4	19931105		
PRIORITY APPLN. INFO.:			JP 1986-132473	19860607

IT **4058-69-9**
RL: USES (Uses)
(photothermog. material containing microcapsules of, for improved storage stability)

RN 4058-69-9 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-benzoyloxime (9CI) (CA INDEX NAME)



L31 ANSWER 35 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
GI



I

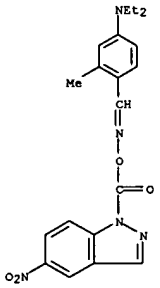
AB A Ag halide photog. material having ≥1 light-sensitive Ag halide emulsion layer contains ≥1 photog. reagent precursor of the formula R1CH:NOCY(LX)mTn(PUG) (R1 = H, other monovalent substituent; Y = O, NR2; R2 = substituent; L = bivalent linkage group; X = electron-attracting center; T = timing group; PUG = photog. useful group having O, N or cyclic structure; n, m = 0, 1). The precursor, which is quite stable during storage of the material, releases the photog. reagent at an appropriate time during its development. It is especially useful for development at low pH, e.g. 9-12, and for dry thermal processing. Thus, development inhibitor precursor I was added to the emulsion layer of an exptl. monocolor photog. film as a coupler/precursor codispersion. Upon exposure and then development by a normal color neg. process, it produced a remarkable reduction in fog without affecting speed or contrast.

ACCESSION NUMBER: 1988:177038 CAPLUS
DOCUMENT NUMBER: 108:177038
TITLE: Timing precursor in silver halide photographic material
INVENTOR(S): Ito, Isamu; Kawada, Ken
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62163051	A2	19870718	JP 1986-4290	19860114
JP 07062757	B4	19950705		
PRIORITY APPLN. INFO.:			JP 1986-4290	19860114

IT **114040-47-0P**
RL: PREP (Preparation)
(preparation of, as timing photog. development inhibitor precursor)
RN 114040-47-0 CAPLUS
CN Benzaldehyde, 4-(diethylamino)-2-methyl-, O-[(5-nitro-1H-indazol-1-yl)carbonyl]oxime (9CI) (CA INDEX NAME)

L31 ANSWER 35 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L31 ANSWER 36 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
GI For diagram(s), see printed CA Issue.
AB Oxime esters I [X = H, alkyl, halo; Z = H, Me; R1 = H, alkyl, alkoxymethyl, -Et, alkylthiomethyl, -Et, cyano, Me (un)substituted cycloalkyl, Ac, Bz, etc.; R2 = H, when R1 ≠ H, R2 = alkyl, alkoxy-, chloro-, azolyl-, dimethoxymethyl, cyano, etc., when R1 = H, Me, or Ac, R2 = (tetrahydro)furyl, thienyl, tetrahydropyranyl, etc.; CR1R2 = cycloalkylidene, cycloalkenylidene, or 4-oxacyclohexadienylidene (un)substituted by Me, with optional O or S atoms in 5- or 6-numbered rings], useful as herbicides (no data), were prepared by reactions of acid halides II (R = halo) with R1R2C:NOH. Me2C:NOH in CH2Cl2 was treated with pyridine, then portionwise with 3,7-dichloro-8-quinolinecarbonyl chloride at 15-20° and the mixture stirred 8 h at 25° to give 81% I (R1 = R2 = Me, X = Cl, Z = H).

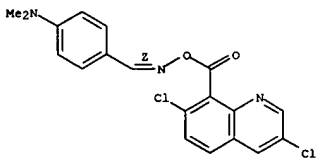
ACCESSION NUMBER: 1987:598109 CAPLUS
DOCUMENT NUMBER: 107:198109
TITLE: Oxime esters of substituted 8-quniolinecarboxylic acids, their preparation, and their use as herbicides
INVENTOR(S): Plath, Peter; Eicken, Karl; Zeeh, Bernd; Eichenauer, Ulrich; Hagen, Helmut; Kohler, Rolf Dieter; Meyer, Norbert; Wuerzer, Bruno
PATENT ASSIGNEE(S): BASF A.-G. , Fed. Rep. Ger.
SOURCE: Ger. Offen., 6 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3545904	A1	19870625	DE 1985-3545904	19851223
JP 62148471	A2	19870702	JP 1986-292645	19861210
EP 230627	A1	19870805	EP 1986-117717	19861219
EP 230627	B1	19920304		
R: BE, CH, DE, FR, GB, IT, LI, NL				
HU 43042	A2	19870928	HU 1986-5383	19861222
HU 198022	B	19890728		
US 4808212	A	19890228	US 1986-944519	19861222
PRIORITY APPLN. INFO.:			DE 1985-3545904 A	19851223

IT **110828-98-3P 110853-36-6P 110853-47-9P 110853-65-1P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide)
RN 110828-98-3 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[(3,7-dichloro-8-quinolinyl)carbonyl]oxime, (Z)- (9CI) (CA INDEX NAME)

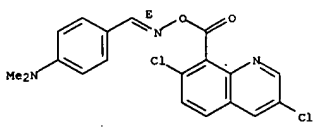
Double bond geometry as shown.

L31 ANSWER 36 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



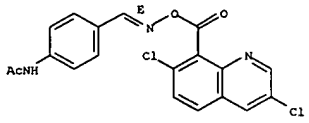
RN 110853-36-6 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[(3,7-dichloro-8-quinolinyl)carbonyl]oxime, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 110853-47-9 CAPLUS
CN Acetamide, N-[4-[[[[(3,7-dichloro-8-quinolinyl)carbonyl]oxy]imino]methyl]phenyl]-, (E)- (9CI) (CA INDEX NAME)

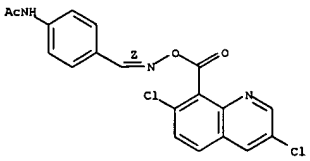
Double bond geometry as shown.



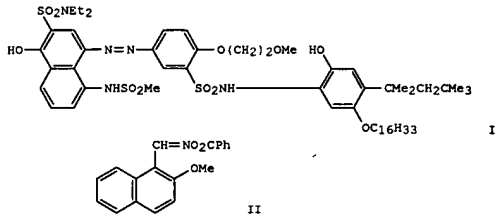
RN 110853-65-1 CAPLUS
CN Acetamide, N-[4-[[[[(3,7-dichloro-8-quinolinyl)carbonyl]oxy]imino]methyl]phenyl]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L31 ANSWER 36 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L31 ANSWER 37 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
GI



I

II

AB Heat-developable photosensitive materials giving an image with a high signal-to-noise ratio, that is a high Dmax and a low Dmin, and a high d. are composed of a photosensitive gelatin-Ag halide emulsion layer, a dye-forming substance that upon reduction at a high temperature produces a diffusible dye, and an organic acid precursor with the structural unit -CH:NO2C- that is very stable at .ltorsim.50°, but frees an acid at temps. proceeding to development to neutralize the base and stop the development. Thus, a PET support was coated with a composition containing a gelatin-Ag(Br,I) emulsion 20, a gelatin-Ag benzotriazole emulsion 10, a dispersion of I 33 g, a 5% aqueous solution of p-C9H19C6H4O(CH2CH2O)10H 10, a 10% aqueous solution of H2NSO2NMe2 4, a gelatin dispersion of II 10 mL, and a solution of guanidine trichloroacetate 1.6 mL in EtOH 16 mL at 33μ (wet). After drying a gelatin protective layer was added. The resultant material was then imagewise exposed 10 s at 2000 lx with a W lamp, heated for 60 s on a 140° heating block, contacted with a wet receptor sheet, and heated 6 s at 80° to give a Dmax of 2.10 and a Dmin of 0.20 vs. 2.35 and 0.85, resp., for a II-free control.

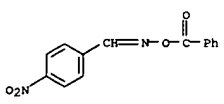
ACCESSION NUMBER: 1986:139353 CAPLUS
DOCUMENT NUMBER: 104:139353
TITLE: Heat-developing light-sensitive color material
INVENTOR(S): Kato, Masatoshi; Kitaguchi, Hiroshi
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd. , Japan
SOURCE: Ger. Offen., 90 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3508761	A1	19850919	DE 1985-3508761	19850312
JP 60192939	A2	19851001	JP 1984-48305	19840314
JP 04069775	B4	19921109		
US 4656126	A	19870407	US 1985-711885	19850314

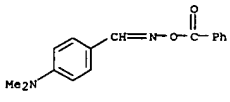
PRIORITY APPLN. INFO.: JP 1984-48305 A 19840314

L31 ANSWER 37 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

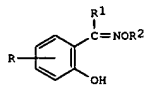
IT **3848-35-9 4058-69-9**
RL: USES (Uses)
(color diffusion-transfer photothermog. materials containing base-neutralizing acid precursor from, for improved image quality)
RN 3848-35-9 CAPLUS
CN Benzaldehyde, 4-nitro-, O-benzoyloxime (9CI) (CA INDEX NAME)



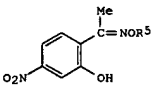
RN 4058-69-9 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-benzoyloxime (9CI) (CA INDEX NAME)



L31 ANSWER 38 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
GI



I



II

AB Aromatic oximes I [R = H, Cl, NO2, CO2Et, CO2Me, CONH2, CN; R1 = H, Me, CN, Ph; R2 = R3CO (R3 = H, C1-10 alkyl, allyl, aralkyl), N-protected amino acid or peptide moiety] were used in the acylation of HNR3R4 [R3 = H, C1-5 alkyl, (un)substituted Ph or CH2Ph; R4 = C1-10 alkyl, allyl, aralkyl, amino acid or peptide moiety] to give amides R2NR3R4. Thus, Z-Gly-OH (Z = PhCH2O2C) was condensed with oxime II (R5 = H) by DCC in DMF to give 87% II (R5 = Z-Gly) (III). PhCH2NH2 was acylated by III to give 80% reaction in 2 min 25 s.

ACCESSION NUMBER: 1985:185507 CAPLUS
DOCUMENT NUMBER: 102:185507
TITLE: Acylation with acylating agent
INVENTOR(S): Hayashi, Ikuo; Ogihara, Keizo; Itikawa, Tadao; Shimizu, Kiyoshi
PATENT ASSIGNEE(S): Nitto Boseki Co., Ltd. , Japan
SOURCE: Eur. Pat. Appl., 17 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

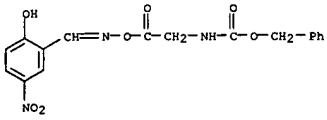
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 127342	A2	19841205	EP 1984-302958	19840502
EP 127342	A3	19870408		
R: CH, DE, FR, GB, LI				
JP 59204156	A2	19841119	JP 1983-78572	19830504
US 4559172	A	19851217	US 1984-605781	19840501

PRIORITY APPLN. INFO.: JP 1983-78572 A 19830504

OTHER SOURCE(S): CASREACT 102:185507

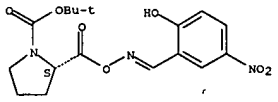
IT **96140-47-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation by, of benzylamines)
RN 96140-47-5 CAPLUS
CN Carbamic acid, [2-[[[(2-hydroxy-5-nitrophenyl)methylene]amino]oxy]-2-oxoethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

L31 ANSWER 38 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

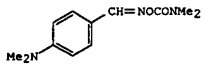


IT **96140-56-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(peptide coupling of, with dipeptide Me ester)
RN 96140-56-6 CAPLUS
CN 1-Pyrrolidinecarboxylic acid, 2-[[[[(2-hydroxy-5-nitrophenyl)methylene]amino]oxy]carbonyl]-, 1,1-dimethylethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



L31 ANSWER 39 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
GI



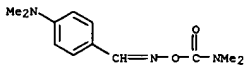
I

AB Photothermog. materials contain in a binder microparticles of a base-releasing precursor which is substantially insol. in water. The materials have good preservation stability due to the precursor having high resistance against self-decomposition by ambient moisture. Thus, a water-insol. type precursor I was mixed with poly(ethylene glycol), gelatin, and water and crushed using a mill to give a dispersion of precursor grains with an average size of 1 μm. The dispersion was then coated on a poly(ethylene terephthalate) support together with a Ag(Br,I) emulsion, a cyan coupler dispersion containing 2-dodecylcarbamoyl-1-naphthol, and 2,6-dichloro-p-aminophenol to form a photosensitive film. The film was imagewise-exposed and heat-developed at 150° for 20 s to give a neg. cyan dye image with Dmax 2.08 and Dmin 0.25.

ACCESSION NUMBER: 1985:123151 CAPLUS
DOCUMENT NUMBER: 102:123151
TITLE: Photothermographic materials
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

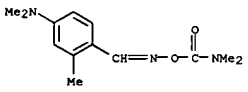
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 59174830	A2	19841003	JP 1983-50000	19830325
JP 03058498	B4	19910905		
US 4514493	A	19850430	US 1984-592197	19840322
PRIORITY APPLN. INFO.:			JP 1983-50000 A	19830325

IT **93369-38-1**
RL: USES (Uses)
(color photothermog. composition containing)
RN 93369-38-1 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[(dimethylamino)carbonyl]oxime (9CI) (CA INDEX NAME)

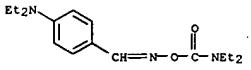


IT **95186-87-1 95186-88-2**
RL: USES (Uses)
(color photothermog. material containing)

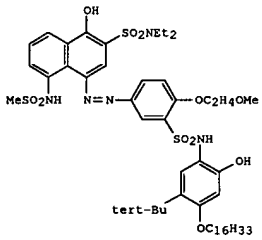
L31 ANSWER 39 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 95186-87-1 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-2-methyl-, O-[(dimethylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



RN 95186-88-2 CAPLUS
CN Benzaldehyde, 4-(diethylamino)-, O-[(diethylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



L31 ANSWER 40 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
GI



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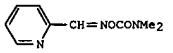


II

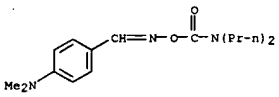
AB A photog. material which forms low-fog storage-stable dye images by heating consists of ≥1 Ag halide emulsion, a binder, a dye-releasing redox compound, and a base precursor RCH:NOCONR1R2 (R = alkyl, cycloalkyl, alkenyl, aryl, aralkyl, acyl, heterocyclyl; R1, R2 = H, alkyl, cycloalkyl, aralkyl, or RR1 together can form a ring, or NRR1 may form an imino group by a double bond. Thus, a poly(ethylene terephthalate) support was coated with a composition containing a Ag(Br,I) emulsion 25, a dye-releasing redox compound dispersion (containing I 5, Na bis(2-ethylhexyl) sulfosuccinate 0.5, tricresyl phosphate 5, 10% aqueous gelatin 100 g, EtOAc 30 mL) 33 g, a 5% aqueous solution of C9H19C6H4-p-O(CH2CH2O)10H 10, a 10% aqueous solution of H2NSO2NMe2 4 mL, and a solution containing the base precursor II 2.5 g in EtOH 20 mL, to a wet thickness of 30 μm, dried, imagewise exposed to 2000 lx for 10 s using W lamp, heated 10 s to 140°, contacted with a H2O-wetted image receiver (consisting of a polyester support containing dispersed TiO2 and a gelatin layer of Me acrylate-N,N,N-trimethyl-N-vinylbenzylammonium chloride copolymer), and heated 6 s at 80°. After separation of the elements a neg. magenta image was obtained on the receiver whch had a Dmax and Dmin of 2.05 and 0.2, resp., vs. 0.03 and 0.03, resp., for a II-free control.

ACCESSION NUMBER: 1985:70099 CAPLUS
DOCUMENT NUMBER: 102:70099
TITLE: Heat-developable color photographic materials
INVENTOR(S): Hirai, Hiroyuki; Kawata, Ken

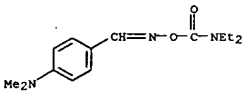
L31 ANSWER 40 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd. , Japan
SOURCE: Eur. Pat. Appl., 61 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 118078	A2	19840912	EP 1984-101801	19840221
EP 118078	A3	19841128		
EP 118078	B1	19880107		
R: DE, FR, GB, NL				
JP 59157637	A2	19840907	JP 1983-31614	19830225
JP 02045180	B4	19901008		
US 4499180	A	19850212	US 1984-583913	19840227
PRIORITY APPLN. INFO.:			JP 1983-31614 A	19830225

IT **94528-51-5**
RL: USES (Uses)
(photog. heat-developable emulsion containing, as base precursor)
RN 94528-51-5 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[(dipropylamino)carbonyl]oxime (9CI) (CA INDEX NAME)

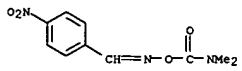


IT **93369-44-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and application of, as base precursor in heat-developable color
photog. materials)
RN 93369-44-9 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[(diethylamino)carbonyl]oxime (9CI) (CA INDEX NAME)

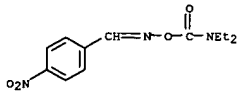


IT **93369-36-9P 93369-37-0P 93369-38-1P**
RL: PREP (Preparation)
(preparation of, for heat-developable color photog. materials)
RN 93369-36-9 CAPLUS

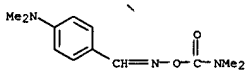
L31 ANSWER 40 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN Benzaldehyde, 4-nitro-, O-[(dimethylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



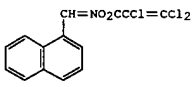
RN 93369-37-0 CAPLUS
CN Benzaldehyde, 4-nitro-, O-[(diethylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



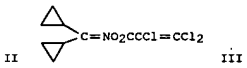
RN 93369-38-1 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[(dimethylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



L31 ANSWER 41 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
GI



II



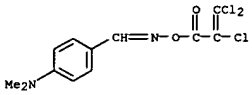
III

AB C12C:CClCO2N:CRR1 (I) (R,R1 = H, lower alkyl, benzyl, cycloalkyl, naphthyl, aryl, etc.) were prepared and shown, in some cases, to be more effective fungicides than kilazin P. Thus, 100 mL PhMe solution containing 40 g
C12C:CClCOCl were added at ≤20° to 30 g PhCH:NOH and 26 g Et3N in 400 mL PhMe, and the mixture was heated 2 h at 50° to give 58 g I (R = Ph, R1 = H). Among 39 other I prepared were I (R,R1 = Me,Me; Me,Et; (RR1=) cyclohexylidene], the naphthyl analog II, and the dicyclopropyl analog III.
ACCESSION NUMBER: 1984:610740 CAPLUS
DOCUMENT NUMBER: 101:210740
TITLE: Trichloroacryloyl oxime derivatives
INVENTOR(S): Yamada, Yasuo; Saito, Junichi; Gotoh, Toshio; Katsumata, Osamu; Sakawa, Shinji
PATENT ASSIGNEE(S): Nihon Tokushu Noyaku Seizo K. K. , Japan
SOURCE: Eur. Pat. Appl., 34 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

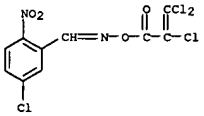
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 112524	A1	19840704	EP 1983-112276	19831207
EP 112524	B1	19860528		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL				
JP 59110665	A2	19840626	JP 1982-220165	19821217
US 4581365	A	19860408	US 1983-557688	19831202
IL 70443	A1	19870130	IL 1983-70443	19831214
BR 8306913	A	19840724	BR 1983-6913	19831215
ZA 8309329	A	19840829	ZA 1983-9329	19831215
DK 8305810	A	19840618	DK 1983-5810	19831216
AU 8322504	A1	19840621	AU 1983-22504	19831219
PRIORITY APPLN. INFO.:			JP 1982-220165 A	19821217

OTHER SOURCE(S): CASREACT 101:210740
IT **93033-19-3P 93033-27-3P 93033-52-4P 93033-53-5P 93033-54-6P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as fungicide)
RN 93033-19-3 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(2,3,3-trichloro-1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)

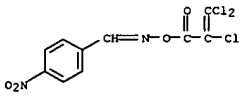
L31 ANSWER 41 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



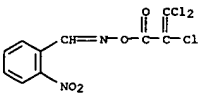
RN 93033-27-3 CAPLUS
CN Benzaldehyde, 5-chloro-2-nitro-, O-(2,3,3-trichloro-1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)



RN 93033-52-4 CAPLUS
CN Benzaldehyde, 4-nitro-, O-(2,3,3-trichloro-1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)

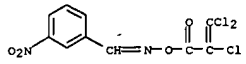


RN 93033-53-5 CAPLUS
CN Benzaldehyde, 2-nitro-, O-(2,3,3-trichloro-1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)



RN 93033-54-6 CAPLUS
CN Benzaldehyde, 3-nitro-, O-(2,3,3-trichloro-1-oxo-2-propenyl)oxime (9CI) (CA INDEX NAME)

L31 ANSWER 41 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L31 ANSWER 42 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
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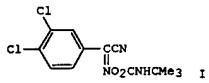


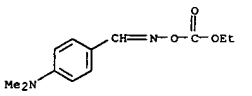
AB Oxime carbamates and oxime carbonates ArC(:NO2CR)X (Ar = substituted Ph, naphthyl, furan, or thiophene; R = mono- or disubstituted amine, substituted alkoxy, substituted alkylthio, the substituents of which include substituted hydrocarbyl and heterocyclic groups; X = H, CN, CO2H, alkyl, alkanoyl, etc.) were prepared and evaluated as antidotes for the protection of crops against triazine, haloacetanilide, and [(pyridyloxy)phenoxy]propionate herbicides. Thus, in preemergence tests with sorghum-millet var Funk G-522, the title compound I (ArC(:NO2CR)X; Ar = 2,4-Cl2C6H4, R = NHCMe3, X = CN) [71059-14-8] at 1.0 ppm offered marked protection against Metolachlor [51218-45-2] at 5 ppm. Dust, granulate, wettable powder, and emulsifiable concentrate formulations for antidotes are described.

ACCESSION NUMBER: 1984:419085 CAPLUS
DOCUMENT NUMBER: 101:19085
TITLE: 3,4-Dichlorophenylacetonitrile-N-tert-butylcarbamoyloxy ether for the protection of crops against injury by herbicides
INVENTOR(S): Martin, Henry
PATENT ASSIGNEE(S): Ciba-Geigy Corp. , USA
SOURCE: U.S., 17 pp. Cont. of U.S. Ser. No. 938,205, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4416686	A	19831122	US 1980-112049	19800114
US 4426221	A	19840117	US 1982-425812	19820928
US 4453969	A	19840612	US 1982-425814	19820928
US 4453974	A	19840612	US 1982-425815	19820928
US 4456468	A	19840626	US 1982-425813	19820928
US 4475945	A	19841009	US 1982-425782	19820928
PRIORITY APPLN. INFO.:			US 1978-938205	A1 19780830
			US 1980-112049	A3 19800114

OTHER SOURCE(S): CASREACT 101:19085
IT **71063-92-8P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide antidote)

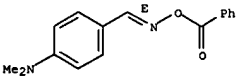
L31 ANSWER 42 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 71063-92-8 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(ethoxycarbonyl)oxime (9CI) (CA INDEX NAME)



L31 ANSWER 43 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB The rate of E-Z isomerization of O-acylaldoximes in glacial HOAc has been followed by using spectral data. The decrease of O-acylaldoxime with time was established from the decrease of the limit current of the polarog. wave. Gas chromatog. and liquid chromatog. were applied to determine the concentration of the reaction products. The O-acylaldoximes also undergo acid-catalyzed cleavage to give nitriles.

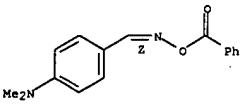
ACCESSION NUMBER: 1984:102525 CAPLUS
DOCUMENT NUMBER: 100:102525
TITLE: Kinetics of reactions of O-benzoylbenzaldoxime derivatives in acetic acid
AUTHOR(S): Mollin, J.; Holakovska, A.
CORPORATE SOURCE: Fac. Nat. Sci., Palacky Univ., Olomouc, CS-771 46, Czech.
SOURCE: Chemicke Zvesti (1983), 37(5), 633-8
CODEN: CHZVAN; ISSN: 0366-6352
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **16061-99-7 88997-13-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(isomerization and cleavage reactions of, in acid medium, kinetics of)
RN 16061-99-7 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-benzoyloxime, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 88997-13-1 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-benzoyloxime, (Z)- (9CI) (CA INDEX NAME)

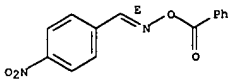
Double bond geometry as shown.



IT **16061-94-2 18322-89-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(isomerization and reactions of, in acid medium, kinetics of)
RN 16061-94-2 CAPLUS
CN Benzaldehyde, 4-nitro-, O-benzoyloxime, (E)- (9CI) (CA INDEX NAME)

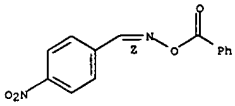
Double bond geometry as shown.

L31 ANSWER 43 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



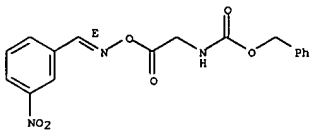
RN 18322-89-9 CAPLUS
CN Benzaldehyde, 4-nitro-, O-benzoyloxime, [C(Z)]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

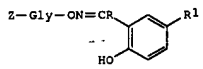


L31 ANSWER 44 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Double bond geometry as shown.



L31 ANSWER 44 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
GI

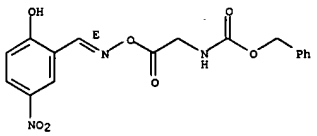


I

AB Title esters I (Z = PhCH2O2C; R = H, Me, Ph; R1 = H, Cl, NO2) were prepared
by several methods. For aminolysis with benzylamine, esters I showed higher reactivity than similar esters containing no o-HO group. This is attributed to formation of an intramol. H bond between the o-HO group and the hydroxyimino N. This mechanism of activation seems to be an intramol.
acid-catalysis. I (R = H) were the most reactive. The reactivity of esters I is also discussed in relation to pKa values of aromatic o-hydroxy
oximes.

ACCESSION NUMBER: 1984:7101 CAPLUS
DOCUMENT NUMBER: 100:7101
TITLE: Reactivity of aromatic o-hydroxy oximes. I. Synthesis and aminolysis of acylglycine esters of aromatic o-hydroxy oximes
AUTHOR(S): Hayashi, Ikuo; Ogihara, Keizo; Shimizu, Kiyoshi
CORPORATE SOURCE: Res. Dev. Lab., Nitto Boseki Co., Ltd., Koriyama, 963,
Japan
SOURCE: Bulletin of the Chemical Society of Japan (1983), 56(8), 2432-7
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **87974-60-5P 87974-69-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and aminolysis of)
RN 87974-60-5 CAPLUS
CN Carbamic acid, [2-[[[(2-hydroxy-5-nitrophenyl)methylene]amino]oxy]-2-oxoethyl]-, phenylmethyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

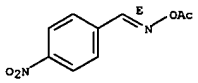


RN 87974-69-4 CAPLUS
CN Carbamic acid, [2-[[[(3-nitrophenyl)methylene]amino]oxy]-2-oxoethyl]-, phenylmethyl ester, (E)- (9CI) (CA INDEX NAME)

L31 ANSWER 45 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB The CTAB micelle-catalyzed reaction of RCH:NOH (I; R = aryl) with p-AcOC6H4NO2 to give RCH:NOAc was studied. The catalysis is more effective as the base strength of I decreases, but the reactivity of I is not dependent on its basicity. These are orbital controlled reactions involving interactions between both the n and π occupied orbitals of I and the LUMO of p-AcOC6H4NO2.

ACCESSION NUMBER: 1982:5759 CAPLUS
DOCUMENT NUMBER: 96:5759
TITLE: Effects of micelles on the basicity and reactivity of α-aromatic nucleophiles
AUTHOR(S): Meyer, G.; Viout, P.
CORPORATE SOURCE: Groupe Rech. 12, CNRS, Thiais, 94320, Fr.
SOURCE: Tetrahedron (1981), 37(12), 2269-72
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: French
IT **80055-47-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of, micelle effect on)
RN 80055-47-6 CAPLUS
CN Benzaldehyde, 4-nitro-, O-acetyloxime, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L31 ANSWER 46 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN

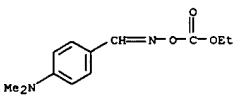
AB Carbamates RR1C:NO2CR2 [I; R = optionally substituted Ph or naphthyl, esterified CO2H, optionally substituted carbamoyl; R1 = cyano, alkanoyl, CO2H, esterified CO2H, H, halo, alkyl, optionally carbamoyl; R2 = optionally substituted NH2, ZR3 (Z = O, S; R3 = aliphatic, cycloaliph. araliph., aromatic, or heterocyclic group)] were prepared; they showed usefulness as antidotes for herbicides. Thus, I (R = 3,4-Cl2C6H3, R1 = cyano, R2 = SEt) was prepared in 73.7% yield by treating 3,4-Cl2C6H3C(:NOH)CN with EtSCOCl.

ACCESSION NUMBER: 1981:442679 CAPLUS
DOCUMENT NUMBER: 95:42679
TITLE: Oxime carbamates and -carbonates for the protection of plant cultures
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: Neth. Appl., 54 pp.
CODEN: NAXXAN
DOCUMENT TYPE: Patent
LANGUAGE: Dutch
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 7808962	A	19800304	NL 1978-8962	19780831
PRIORITY APPLN. INFO.:			NL 1978-8962 A	19780831

IT **71063-92-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 71063-92-8 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(ethoxycarbonyl)oxime (9CI) (CA INDEX NAME)



L31 ANSWER 47 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN

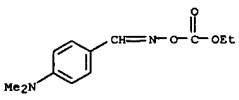
AB The title compds. RCR1:NOR2 [R = (un)substituted Ph, naphthyl, furyl, or thienyl, or carboxylic ester or carbamyl group; R1 = cyano, alkanoyl, carboxylic ester, CO2H, halo, H, carboxamide, alkyl; R2 = carboxamide, ester, thioester group], useful as antidotes for protecting cultivated plants from harmful agrochems., especially herbicides, were prepared The compds.
are especially useful in seed or seedling dressing compns. E.g., PhC(CN):NO2CNHMe was prepared (89.8%) by treating benzyl cyanide oxime with
MeNCO in the presence of diazabicyclooctane catalyst (MeCN, 50°).

ACCESSION NUMBER: 1981:46990 CAPLUS
DOCUMENT NUMBER: 94:46990
TITLE: Oxime carbamates and oxime carbonates for the protection of cultivated crops
INVENTOR(S): Martin, Henry
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: Brit. UK Pat. Appl., 21 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2028797	A	19800312	GB 1978-35200	19780831
GB 2028797	B2	19830427		
PRIORITY APPLN. INFO.:			GB 1978-35200 A	19780831

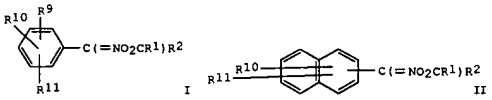
IT **71063-92-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide antidote)

RN 71063-92-8 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(ethoxycarbonyl)oxime (9CI) (CA INDEX NAME)



L31 ANSWER 48 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN

GI



AB Glyoxylonitrile oximes and similar compds. were O-acylated by organic isocyanates, carbamoyl chlorides, chloroformate esters, and esters of ClC(O)SH to yield RC(:NO2CR1)R2 [R = CO2R3 (R3 = aliphatic, cycloaliph., or araliph. group), COR4 [R4 = NR5R6 (R5 = H, alkyl, cycloalkyl; R6 = H, aliphatic, cycloaliph., araliph., aromatic, or heterocyclic group; or NR5R6 form a heterocycle), NHCONHR6 (R6 same as above)], furyl, thienyl, halofuryl or -thienyl, nitrofuryl or -thienyl, alkylfuryl or -thienyl; R1 = NR7R8 (R7 = H, alkoxy, aliphatic, cycloaliph., araliph., aromatic, or heterocyclic group; R8 = aliphatic, cycloaliph., araliph., aromatic, or heterocyclic group), ZR8 (Z = O or S, R8 same as above); R2 = cyano, alkanoyl, (un)esterified CO2H, H, carbamoyl, halo, alkyl] and aromatic compds. I and II (R1 and R2 same as above; R9 = H, halo, alkyl, alkoxy, phenoxy; R10 and R11 independently are H, halo, NO2, alkyl, haloalkyl, alkoxy), which showed effectiveness as antidotes for herbicides. A mixture of PhC(:NOH)CN, MeNCO, and diazabicyclooctane in MeCN was heated at 50° to give PhC(:NO2CNHMe)CN.

ACCESSION NUMBER: 1981:30218 CAPLUS
DOCUMENT NUMBER: 94:30218
TITLE: Oxime carbamates and oxime carbonates useful in protecting plants
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: Fr. Demande, 44 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

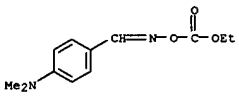
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2434802	A1	19800328	FR 1978-25043	19780830
FR 2434802	B1	19810306		
PRIORITY APPLN. INFO.:			FR 1978-25043 A	19780830

IT **71063-92-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 71063-92-8 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(ethoxycarbonyl)oxime (9CI) (CA

L31 ANSWER 48 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

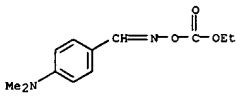
NAME)



L31 ANSWER 49 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB RR1C:NO2CR2 (R = optionally substituted Ph, naphthyl, thienyl, furyl; R1 =
cyano, alkanoyl, optionally esterified or amidated CO2H, H, halogen, alkyl; R2 = amino, optionally etherified OH or SH) were prepared Thus NCCPh:NOH was treated with MeNCS to give 89.8% NCCPh:NO2CNHMe. Wheat seeds treated with 10 ppm PhMeC:NO2CNHC6H4Cl-4 (I) showed .apprx.30% damage when grown in soil pretreated with 8 ppm Me 2-[4-(3,5-dichloro-2-pyridyloxy)phenoxy]propionate, compared with .apprx.70% damage in the absence of treatment with I.
ACCESSION NUMBER: 1980:586009 CAPLUS
DOCUMENT NUMBER: 93:186009
TITLE: Oxime carbonates useful in protecting plants from damage by herbicides
INVENTOR(S): Martin, Henry
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: Braz. Pedido PI, 59 pp.
CODEN: BPXXDX
DOCUMENT TYPE: Patent
LANGUAGE: Portuguese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

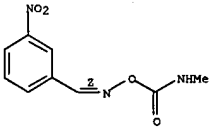
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BR 7805666	A	19800318	BR 1978-5666	19780831
PRIORITY APPLN. INFO.:			BR 1978-5666 A	19780831

IT **71063-92-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 71063-92-8 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(ethoxycarbonyl)oxime (9CI) (CA INDEX NAME)



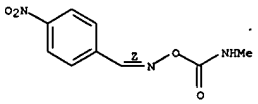
L31 ANSWER 50 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB Hydrolysis of R2C6H4CR1:NO2CNRMe (R, R1 = H, Me; R2 = H, Me, MeO, Me2CH, Br, m- and p-O2N), studied in 0.01-5.0 N OH- at 25° showed 1st-order dependence each in OH- and the ester. The data suggest an E1cB elimination mechanism with formation of an isocyanate intermediate. The Hammett ρ values were different from those usually reported for such a reaction scheme, as the imine bond weakens the substituent effects.
ACCESSION NUMBER: 1980:407484 CAPLUS
DOCUMENT NUMBER: 93:7484
TITLE: Kinetics and mechanism of hydrolysis of insecticidal O-(methylcarbamoyl)oximes
AUTHOR(S): Mrlina, Georges; Calmon, Jean Pierre
CORPORATE SOURCE: Lab. Chim. Org. Biol. Physicochem. Sol, Ec. Natl. Super. Agron., Toulouse, 31076, Fr.
SOURCE: Journal of Agricultural and Food Chemistry (1980), 28(3), 605-9
CODEN: JAFCAU; ISSN: 0021-8561
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **73744-22-6P 73744-23-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and alkaline hydrolysis of, kinetics of)
RN 73744-22-6 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[(methylamino)carbonyl]oxime, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

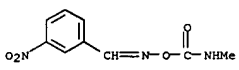


RN 73744-23-7 CAPLUS
CN Benzaldehyde, 4-nitro-, O-[(methylamino)carbonyl]oxime, (Z)- (9CI) (CA INDEX NAME)

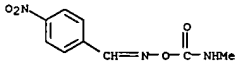
Double bond geometry as shown.



L31 ANSWER 51 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB As the anticholinesterase activity and the mechanism of alkaline hydrolysis of
O-(methylcarbamoyl) benzaldoximes and acetophenoximes are analogous to those of Ph N-methylcarbamates, these 2 groups of derivs. were compared by
means of structure-activity relations. The correlations with the electronic substituent parameter σ showed that the mechanism of inhibition of acetylcholinesterase [9000-81-1] by O-(methylcarbamoyl) oximes is the same as that observed for Ph N-methylcarbamates bearing strongly electron-withdrawing substituents. The correlations with the bimol. rate constant kOH suggest that the mechanism of the alkaline hydrolysis
of oxime carbamates may closely parallel their mechanism of interaction with acetylcholinesterase at the serine hydroxyl.
ACCESSION NUMBER: 1980:210126 CAPLUS
DOCUMENT NUMBER: 92:210126
TITLE: Inhibition of acetylcholinesterase by O-(methylcarbamoyl) oximes. Structure-activity relationships
AUTHOR(S): Mrlina, Georges; Calmon, Jean Pierre
CORPORATE SOURCE: Lab. Chim. Org. Biol. Phys.-Chim. Sol, Ec. Natl. Super. Agron., Toulouse, 31076, Fr.
SOURCE: Journal of Agricultural and Food Chemistry (1980), 28(3), 673-5
CODEN: JAFCAU; ISSN: 0021-8561
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **39102-00-6 39102-02-8**
RL: BIOL (Biological study)
(acetylcholinesterase inhibition by)
RN 39102-00-6 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



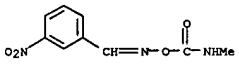
RN 39102-02-8 CAPLUS
CN Benzaldehyde, 4-nitro-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



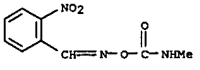
L31 ANSWER 52 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB The oxime carbamates and carbonates ArCX(:NOCOR) (Ar = substituted or unsubstituted Ph, naphthyl, 2-furanyl, H2NCO, MeOCO, EtOCO, etc.; X = CN, Me, NO2, etc.; R = substituted NH2, alkoxy, alkylthio, etc.) are herbicidal antidotes. Thus, in a pre-emergence laboratory experiment, 1 ppm
PhC(CN)(:NOCONHPr-iso) [71059-03-5] protected sorghum millet against the phytotoxic effect of metolachlor [51218-45-2]. The synthesis of the compds. is given.
ACCESSION NUMBER: 1980:141801 CAPLUS
DOCUMENT NUMBER: 92:141801
TITLE: Oxime carbamates and oxime carbonates for the protection of cultivated crops
INVENTOR(S): Martin, Henry
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: S. African, 56 pp.
CODEN: SFXXAB
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ZA 7804846	A	19790829	ZA 1978-4846	19780825
DE 2837204	A1	19800306	DE 1978-2837204	19780825
DE 2837204	C2	19891026		
CA 1159071	A1	19831220	CA 1978-310206	19780829
AU 530210	B2	19830707	AU 1978-39380	19780830
AU 7839380	A1	19800306		
PRIORITY APPLN. INFO.:			ZA 1978-4846 A	19780825

IT **39102-00-6 39102-01-7 71063-92-8 72405-73-3**
RL: BIOL (Biological study)
(preparation as herbicide antidote)
RN 39102-00-6 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)

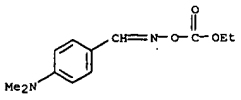


RN 39102-01-7 CAPLUS
CN Benzaldehyde, 2-nitro-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)

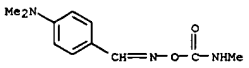


RN 71063-92-8 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(ethoxycarbonyl)oxime (9CI) (CA INDEX

L31 ANSWER 52 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
NAME)



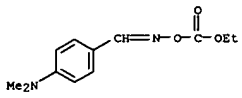
RN 72405-73-3 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



L31 ANSWER 53 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB ArC[:NOC(O)R]R1 [Ar = CO2R2 (R2 = alkyl, cycloalkyl, aralkyl), substituted carbamoyl, Ph, halo-, alkyl-, alkoxy-, phenoxy-, cyano-, nitro-, (haloalkyl)-, or (trifluoromethyl)phenyl, naphthyl, halo-, nitro-, alkyl-, (haloalkyl)-, or alkoxynaphthyl; R = NR3R4 (R3 = H, alkoxy; R4 = alkyl, cycloalkyl, aralkyl, aryl, heteroaryl), ZR4 (Z = O, S; R4 same as above); R1 = cyano, alkanoyl, carbalkoxy, CO2H, H, carbamoyl, halo, alkyl] were prepared by different methods and they protected plants against herbicides.
Thus, MeNCO and diazabicyclooctane was added to PhC(:NOH)CN in MeCN, and the mixture was heated at 50° to give PhC(:NO2CNHMe)CN.
ACCESSION NUMBER: 1979:507670 CAPLUS
DOCUMENT NUMBER: 91:107670
TITLE: (Hydroximino)malonic acid carbamates and carbonates for protecting plants from herbicides
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: Belg., 45 pp.
CODEN: BEXXAL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

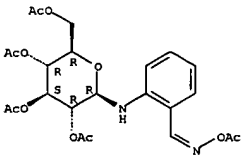
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 870066	A1	19790228	BE 1978-190145	19780830
PRIORITY APPLN. INFO.:			BE 1978-190145 A	19780830

IT **71063-92-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 71063-92-8 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(ethoxycarbonyl)oxime (9CI) (CA INDEX NAME)



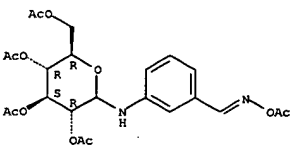
L31 ANSWER 54 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB N-glycosides of o-H2NC6H4CH:NOH with D-glucose, D-galactose, D-mannose, L-rhamnose, and D-ribose were prepared by fusing the reactants in the presence of aqueous HCl. N-glycosides of m-H2NC6H4CH:NOH were prepared similarly. All glycosides in the meta series are colorless, whereas those in the ortho series are bright yellow due to formation of a pseudonitroso system. The α-anomer structure is presumed for the ortho derivs., whereas the β-anomers predominate in the meta series.
ACCESSION NUMBER: 1979:39181 CAPLUS
DOCUMENT NUMBER: 90:39181
TITLE: Syntheses and studies on N-glycosides. VII. N-Glycosides of o- and m-aminobenzaldoximes
AUTHOR(S): Sykulski, Jerzy; Czyzewska, Joanna
CORPORATE SOURCE: Sch. Med., Inst. Basic Chem. Sci., Lodz, Pol.
SOURCE: Acta Poloniae Pharmaceutica (1978), 35(2), 169-73
CODEN: APPHAX; ISSN: 0001-6837
DOCUMENT TYPE: Journal
LANGUAGE: Polish
IT **68768-60-5P 68768-61-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 68768-60-5 CAPLUS
CN Benzaldehyde, 2-[(2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)amino]-, 1-(O-acetyloxime) (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



RN 68768-61-6 CAPLUS
CN Benzaldehyde, 3-[(2,3,4,6-tetra-O-acetyl-D-glucopyranosyl)amino]-, 1-(O-acetyloxime) (9CI) (CA INDEX NAME)

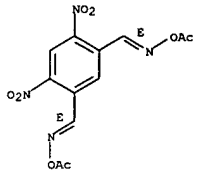
Absolute stereochemistry.
Double bond geometry unknown.



L31 ANSWER 54 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

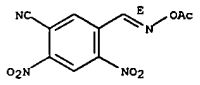
L31 ANSWER 55 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB The reaction of 4,6-dinitroisophthalaldehyde with pyridine gave 1-(2,4-diformyl-5-hydroxyphenyl)pyridinium hydroxide inner salt (I), and the reaction of 4,6-dinitroisophthalonitrile with pyridine gave the 2,4-dicyano analog of I as the main product, with 1-(3,5-dicyano-2-hydroxy-6-nitrophenyl)pyridinium hydroxide inner salt and 4-hydroxy-6-nitroisophthalonitrile as side products.
ACCESSION NUMBER: 1978:529220 CAPLUS
DOCUMENT NUMBER: 89:129220
TITLE: The reaction of 4,6-dinitroisophthalaldehyde and 4,6-dinitroisophthalonitrile with pyridine
AUTHOR(S): Adam, Jean Marie; Hindermann, Peter; Winkler, Tammo
CORPORATE SOURCE: Farbenforschungslab., Ciba-Geigy A.-G., Basel, Switz.
SOURCE: Helvetica Chimica Acta (1978), 61(5), 1778-83
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 89:129220
IT **67640-45-3P 67640-47-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 67640-45-3 CAPLUS
CN 1,3-Benzenedicarboxaldehyde, 4,6-dinitro-, bis(O-acetyloxime), (E,E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



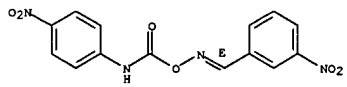
RN 67640-47-5 CAPLUS
CN Benzonitrile, 5-[[(acetyloxy)imino]methyl]-2,4-dinitro-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



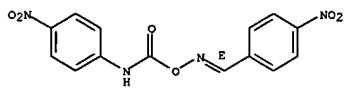
L31 ANSWER 56 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB The alkaline hydrolysis kinetics and mechanism of 4-O2NC6H4NRCO2N:CHC6H4R1 (I; R = H, Me; R1 = H, 4-MeO, 4-Me, 3-Cl, 3-NO2, 4-NO2) were determined I (R = H) in aqueous EtOH containing NaOH gave 4-O2NC6H4NHCO2Na (which decomposed to 4-O2NC6H4NH2) and RC6H4CH:NONa (II; R = H, 4-MeO, 4-Me, 3-Cl, 3-NO2, 4-NO2) via an ElcB mechanism; II hydrolyzed to give the corresponding RC6H4CHO. The hydrolysis of I (R = H) exhibited ρ 1.4 and β-1.4. The hydrolysis of I (R = Me) gave 4-O2NC6H4NHMe and the corresponding II via a BAc2 mechanism in which N-C bond cleavage occurred in the rate-determining decomposition of the tetrahedral intermediate; this process had ρ 0.
ACCESSION NUMBER: 1978:104467 CAPLUS
DOCUMENT NUMBER: 88:104467
TITLE: Carbamates. Part IX. Kinetics and mechanism of alkaline hydrolysis of (E)-O-(N-4-nitrophenylcarbamoyl)benzaldoximes in 30% aqueous ethanol
AUTHOR(S): Hladka, J.; Mindl, J.; Vecera, M.
CORPORATE SOURCE: Org. Chem. Dep., Inst. Chem. Technol., Pardubice, Czech.
SOURCE: Collection of Czechoslovak Chemical Communications (1977), 42(11), 3316-24
CODEN: CCCCAK; ISSN: 0366-547X
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **65786-04-1 65786-05-2 65786-08-5**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(solvolysis of, kinetics and mechanism of)
RN 65786-04-1 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[[(4-nitrophenyl)amino]carbonyl]oxime, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 65786-05-2 CAPLUS
CN Benzaldehyde, 4-nitro-, O-[[(4-nitrophenyl)amino]carbonyl]oxime, (E)- (9CI) (CA INDEX NAME)

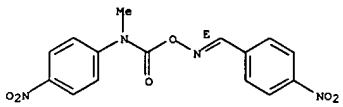
Double bond geometry as shown.



L31 ANSWER 56 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

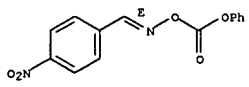
RN 65786-08-5 CAPLUS
CN Benzaldehyde, 4-nitro-, O-[[methyl(4-nitrophenyl)amino]carbonyl]oxime, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L31 ANSWER 57 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB The pyrolysis of (E)-p-RC6H4CH:NOCO2C6H4R1 at 100-20° to give nitriles followed 1st order kinetics and the decomposition rates showed little dependence on inductive effects or solvent polarity. Low entropy values along with the fact that the E and Z-isomers behaved quite differently led to the proposal of a cyclic transition state for the decompns.
ACCESSION NUMBER: 1976:89302 CAPLUS
DOCUMENT NUMBER: 84:89302
TITLE: The mechanism for the thermal decomposition of E-aldoxime carbonates
AUTHOR(S): Prokipcak, J. M.; Forte, P. A.
CORPORATE SOURCE: Dep. Chem., Univ. Guelph, Guelph, ON, Can.
SOURCE: Canadian Journal of Chemistry (1975), 53(22), 3481-6
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **58539-31-4**
RL: PRP (Properties)
(thermodecompn. of, kinetics of)
RN 58539-31-4 CAPLUS
CN Benzaldehyde, 4-nitro-, O-(phenoxycarbonyl)oxime, (E)- (9CI) (CA INDEX NAME)

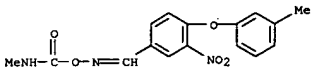
Double bond geometry as shown.



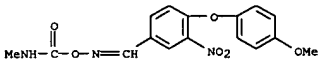
L31 ANSWER 58 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
GI For diagram(s), see printed CA Issue.
AB Diphenyl ether derivs. (I; R = lower alkyl; R1 to R4 = H, halo, lower alkyl, lower alkoxy; n = 0-1; a, b = 0-1; a + b = 1-2) were prepared by reaction of II with RNCO or RNHCOCl. I had insecticidal, anticarcinogenic, and antibacterial activities. Thus, 6.0 g MeNCO and trace Et3N were added to 30.0 g p-(2-nitro-4-chlorophenoxy)benzaldehyde in THF and the mixture refluxed 1 hr to give 27.5 g O-methylcarbamoyl-p-(2-nitro-4-chlorophenoxy)benzaldoxime. Among 13 more I prepared were O-methylcarbamoyl-3-nitro-4-(m-tolyloxy)-, O-methylcarbamoyl-3-nitro-4-(p-methoxyphenoxy)-, O-methylcarbamoyl-3-nitro-4-phenoxy-, and O-methylcarbamoyl-3-nitro-4-(o-chlorophenoxy)benzaldoximes.
ACCESSION NUMBER: 1975:458415 CAPLUS
DOCUMENT NUMBER: 83:58415
TITLE: Diphenyl ether derivatives
INVENTOR(S): Kotani, Akeshi; Inamasu, Shuji
PATENT ASSIGNEE(S): Yoshitomi Pharmaceutical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 50012047	A2	19750207	JP 1973-62203	19730601
PRIORITY APPLN. INFO.:			JP 1973-62203 A	19730601

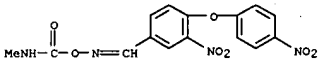
IT **56135-51-4P 56135-52-5P 56135-53-6P 56135-54-7P 56135-55-8P 56135-56-9P 56135-57-0P 56135-61-6P 56135-62-7P 56135-63-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 56135-51-4 CAPLUS
CN Benzaldehyde, 4-(3-methylphenoxy)-3-nitro-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



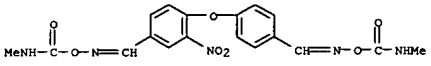
RN 56135-52-5 CAPLUS
CN Benzaldehyde, 4-(4-methoxyphenoxy)-3-nitro-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



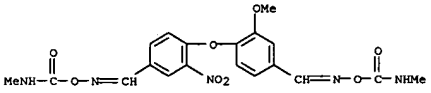
L31 ANSWER 58 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



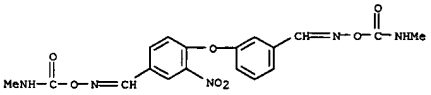
RN 56135-61-6 CAPLUS
CN Benzaldehyde, 4-[4-[[[[(methylamino)carbonyl]oxy]imino]methyl]phenoxy]-3-nitro-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



RN 56135-62-7 CAPLUS
CN Benzaldehyde, 3-methoxy-4-[4-[[[[(methylamino)carbonyl]oxy]imino]methyl]-2-nitrophenoxy]-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)

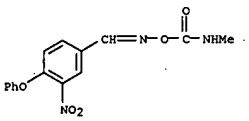


RN 56135-63-8 CAPLUS
CN Benzaldehyde, 4-[3-[[[[(methylamino)carbonyl]oxy]imino]methyl]phenoxy]-3-nitro-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)

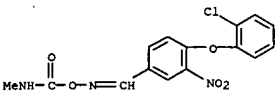


L31 ANSWER 58 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

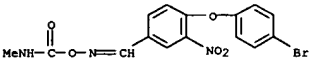
RN 56135-53-6 CAPLUS
CN Benzaldehyde, 3-nitro-4-phenoxy-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



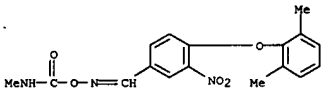
RN 56135-54-7 CAPLUS
CN Benzaldehyde, 4-(2-chlorophenoxy)-3-nitro-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



RN 56135-55-8 CAPLUS
CN Benzaldehyde, 4-(4-bromophenoxy)-3-nitro-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



RN 56135-56-9 CAPLUS
CN Benzaldehyde, 4-(2,6-dimethylphenoxy)-3-nitro-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



RN 56135-57-0 CAPLUS
CN Benzaldehyde, 3-nitro-4-(4-nitrophenoxy)-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)

L31 ANSWER 59 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
GI For diagram(s), see printed CA Issue.
AB Twenty-three mixts. of the oximes I [R = R1 = R2 = Me, R3 = Cl, R4 = H (II)] or III [R = Me, R1 = iodine (IV)] with each other, with other I (R = Me, H, or Ph; R1 = Ph, Me2CHCH2, or 3-02NC6H4; or RR1 = CH:CMeCH2CMe2CH2; R2 = H or Me, R3 = Cl or Me, R4 = H or Cl) or III (R = Me, MeCHEt, or Me2CH; R1 = iodine, Cl or Br) or with 3-RCONHC6H4O2CNR1R2 (R = MeO or Me2N, R1 = H or Me, R2 = CHMeEt, CMe3, CHMeCHMe2, or Ph) or NCCH2OC6H2R2CN-2,6,4 (R = iodine, Br, or Cl), e.g. acetone O-[2-(2,4-dichlorophenoxy)propionyl]oxime-isopropylideneamino 4-cyano-2,6-diiodophenyl carbonate mixture (II-IV mixture) [54841-89-3] had higher herbicidal effects than the components.
ACCESSION NUMBER: 1975:134031 CAPLUS
DOCUMENT NUMBER: 82:134031
TITLE: Herbicidal mixtures
INVENTOR(S): Boroschewski, Gerhard; Puttner, Reinhold; Arndt, Friedrich
PATENT ASSIGNEE(S): Schering A.-G.
SOURCE: Ger. Offen., 50 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2303336	A1	19740725	DE 1973-2303336	19730120
DD 107571	C	19740812	DD 1973-175058	19731203
CS 178442	P	19770915	CS 1973-5704	19731210
CS 178438	P	19770915	CS 1973-8535	19731210
NO 141777	B	19800204	NO 1973-4775	19731214
NO 141777	C	19800521		
PL 91646	P	19770331	PL 1974-168032	19740110
FI 56472	B	19791031	FI 1974-115	19740116
FI 56472	C	19800211		
AU 7464605	A1	19750717	AU 1974-64605	19740117
BE 809928	A1	19740718	BE 1974-139973	19740118
NL 7400739	A	19740723	NL 1974-739	19740118
FR 2214407	A1	19740819	FR 1974-1727	19740118
ZA 7400396	A	19741127	ZA 1974-396	19740118
CH 584505	A	19770215	CH 1974-707	19740118
HU 170900	P	19770928	HU 1974-SC459	19740118
SU 580797	D	19771115	SU 1974-1991123	19740118
SE 401075	B	19780424	SE 1974-666	19740118
SE 401075	C	19780803		
RO 68496	B	19790815	RO 1974-77325	19740118
RO 68496	P	19800115		
RO 69339	P	19800715	RO 1974-84790	19740118
JP 49102842	A2	19740928	JP 1974-9177	19740121
AT 7400466	A	19751115	AT 1974-466	19740121
AT 331555	B	19760825		
GB 1460663	A	19770106	GB 1974-2726	19740121
CA 1013961	A1	19770719	CA 1974-190523	19740121
PL 92143	P	19770331	PL 1974-184009	19740810
SU 667094	D	19790605	SU 1975-2126029	19750418
DK 7502198	A	19750818	DK 1975-2198	19750516
AT 7504032	A	19760215	AT 1975-4032	19750527

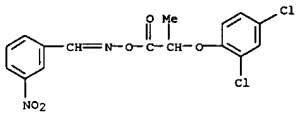
L31 ANSWER 59 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

	AT 333073	B	19761110		
PRIORITY APPLN. INFO.:			DE 1973-2303336	A	19730120
			DK 1973-6311	A	19731122
			AT 1974-466	A	19740121

IT **54842-02-3**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
(herbicide)
RN 54842-02-3 CAPLUS
CN Benzonitrile, 3,5-diiodo-4-[[[[(1-methylethylidene)amino]oxy]carbonyl]oxy]-, mixt. with 3-nitrobenzaldehyde O-[2-(2,4-dichlorophenoxy)-1-oxopropyl]oxime (9CI) (CA INDEX NAME)

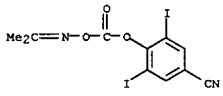
CM 1

CRN 53443-08-6
CMF C16 H12 Cl2 N2 O5



CM 2

CRN 50347-98-3
CMF C11 H8 I2 N2 O3



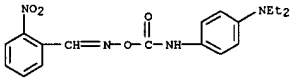
L31 ANSWER 60 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB Compds. obtained by condensation of an oxime with an isocyanate are converted to amines by photolysis or thermolysis. This reaction can be visualized by a dye formation in the presence of a phenolic coupler and an oxidant, the color change of an indicator dye, or by fluorescence emission. Thus, a solution containing PhCH:NOCONH-p-C6H4NEt2, prepared by condensing p-diethylaminophenyl isocyanate with benzdoxime in Et2O, 100, a phenolic coupler 100, m-chloroperbenzoic acid 40 mg, and a 5% poly(Me methacrylate) solution in CH2Cl2 8 ml was coated on a BaSO4-impregnated paper support at 6g/m2, dried, and exposed to a 1 kw uv lamp at 10 cm for 5 sec, or passed through a Thermofax copier to produce a cyan copy.

ACCESSION NUMBER:	1975:92073 CAPLUS
DOCUMENT NUMBER:	82:92073
TITLE:	Recording materials and process
INVENTOR(S):	Mertens, Ludovicus M.
PATENT ASSIGNEE(S):	Agfa-Gevaert
SOURCE:	Belg., 30 pp. CODEN: BEXXAL
DOCUMENT TYPE:	Patent
LANGUAGE:	French
FAMILY ACC. NUM. COUNT:	2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
BE 810213	A2	19740729	BE 1974-1005673		19740128
GB 1458355	A	19761215	GB 1973-4845		19740122
US 3918973	A	19751111	US 1974-437762		19740130
PRIORITY APPLN. INFO.:			GB 1973-4845	A	19730131

IT **54711-46-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 54711-46-5 CAPLUS
CN Benzaldehyde, 2-nitro-, O-[[[4-(diethylamino)phenyl]amino]carbonyl]oxime (9CI) (CA INDEX NAME)



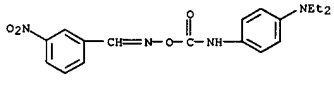
L31 ANSWER 61 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
GI For diagram(s), see printed CA Issue.
AB Compds. R1R2C:NOCONR3R4(R1,R2,R3,R4 = H, alkyl, aryl, or heterocyclic groups) which upon exposure to an arc lamp or to heat liberate an amine capable of undergoing color reactions are used in photog. or thermog. recording compns. The amine precursors are coated with a polymeric binder on a paper or film support. Thus, BaSO4-impregnated paper was coated with 6 g/m2 of a mixture of PhCH:NO-CONHC6H4NEt2-p100, I 100, m-chlorobenzoic acid 40 mg, and a 5% solution of poly(Me methacrylate) in CH2Cl2 8 ml. A 5 sec exposure of the paper to a 1 kW Hg lamp at 10 cm or in a Thermofax copier yielded cyan copies.

ACCESSION NUMBER:	1975:49921 CAPLUS
DOCUMENT NUMBER:	82:49921
TITLE:	Recording with photolytic and/or thermolytic formation of amino compounds
INVENTOR(S):	Mertens, Ludovicus L.
PATENT ASSIGNEE(S):	Agfa-Gevaert A.-G.
SOURCE:	Ger. Offen., 24 pp. CODEN: GWXXBX
DOCUMENT TYPE:	Patent
LANGUAGE:	German
FAMILY ACC. NUM. COUNT:	2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
DE 2403100	A1	19740801	DE 1974-2403100		19740123
GB 1458355	A	19761215	GB 1973-4845		19740122
US 3918973	A	19751111	US 1974-437762		19740130
PRIORITY APPLN. INFO.:			GB 1973-4845	A	19730131

IT **54654-58-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 54654-58-9 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[[[4-(diethylamino)phenyl]amino]carbonyl]oxime (9CI) (CA INDEX NAME)



L31 ANSWER 62 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB Ninety-two ketoxime esters RnC6H5-nOCHR1-CO2N:CR2R3 [I, Rn = 2,4-Cl2, 2,4,5-Cl3, 3-Cl, 2,4-MeCl, 4-Br; R1 = H or Me; R2 = Me, H, Ph, Et, CH2CHMe2, or Pr; R3 =CHMeEt, Me, Ph, CH2CHMe2, C6H4NO2-3, Et, Pr, CHMe2, Bu, CH2OPh, C6H13, or CH2CH2OMe; or R2R3 = CH:CMeCH2CMe2CH2, (CH2)5, CH:CMeCH2CHMeCH2, (CH2)4, or CH2CHMeCH2CH2] were prepared and used for weed control in plant cultures especially in lawn. Thus, addition of 2,4-Cl2C6H3OCH2-COCl to HON:CMeCHMeEt and Et3N in MeCN gave 92% I (Rn = 2,4-Cl2, R1 = H, R2 = Me, R3 = CHMeEt).

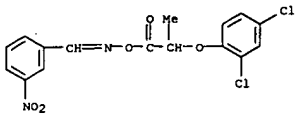
ACCESSION NUMBER:	1974:535752 CAPLUS
DOCUMENT NUMBER:	81:135752
TITLE:	Herbicidal O-phenoxyacetylketoximes
INVENTOR(S):	Nuesslein, Ludwig; Arndt, Friedrich
PATENT ASSIGNEE(S):	Schering A.-G.
SOURCE:	Ger. Offen., 35 pp. CODEN: GWXXBX
DOCUMENT TYPE:	Patent
LANGUAGE:	German
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
DE 2262402	A1	19740801	DE 1972-2262402		19721215
CS 170111	P	19760827	CS 1973-7645		19731107
ES 420904	A1	19760501	ES 1973-420904		19731127
DD 108031	C	19740912	DD 1973-175052		19731203
CH 584510	A	19770215	CH 1973-17131		19731206
FI 55927	C	19791112	FI 1973-3791		19731211
FI 55927	B	19790731			
RO 68556	P	19810830	RO 1973-76956		19731211
FR 2327234	A1	19770506	FR 1973-44534		19731213
FR 2327234	B1	19780324			
BE 808636	A1	19740614	BE 1973-138864		19731214
NL 7317222	A	19740618	NL 1973-17222		19731214
JP 49086539	A2	19740819	JP 1973-140203		19731214
ZA 7309503	A	19741127	ZA 1973-9503		19731214
AT 7310483	A	19750515	AT 1973-10483		19731214
AT 328217	B	19760310			
AU 7363652	A1	19750619	AU 1973-63652		19731214
SU 525417	D	19760815	SU 1973-1978002		19731214
HU 168995	P	19760828	HU 1973-SC457		19731214
PL 91626	P	19770331	PL 1973-167329		19731214
NO 139150	C	19790131	NO 1973-4774		19731214
NO 139150	B	19781009			
GB 1458825	A	19761215	GB 1973-58373		19731217
CA 1013587	A1	19770712	CA 1973-188263		19731217
SU 511853	D	19760425	SU 1974-1998451		19740218
PRIORITY APPLN. INFO.:			DE 1972-2262402	A	19721215

IT **53443-08-6P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and herbicidal activity of)
RN 53443-08-6 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[2-(2,4-dichlorophenoxy)-1-oxopropyl]oxime (9CI)
(CA INDEX NAME)

L31 ANSWER 62 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L31 ANSWER 63 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN

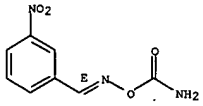
AB The structures assigned to the nitrones prepared from aromatic aldehydes and
soln. of potassium cyanate and hydroxylamine hydrochloride are shown to be incorrect and the deoxygenation reaction ascribed to them spurious. The correct product from the original reaction is demonstrated to be the corresponding O-carbamoyl oxime.

ACCESSION NUMBER: 1974:14448 CAPLUS
DOCUMENT NUMBER: 80:14448
TITLE: O-Carbamoyl oximes
AUTHOR(S): Dalton, David R.; Foley, H. Grant
CORPORATE SOURCE: Dep. Chem., Temple Univ., Philadelphia, PA, USA
SOURCE: Journal of Organic Chemistry (1973), 38(24), 4200-3
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **41514-44-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 41514-44-7 CAPLUS
CN Benzaldehyde, 3-nitro-, O-(aminocarbonyl)oxime, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L31 ANSWER 64 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN

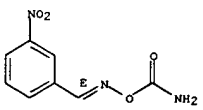
AB RC6H4CHO (R = 4-Br, 4-Cl, 3-O2N) with HONH2.HCl and KOCN gave the O-carbamolyl oximes (E)- RC6H4CH:NOCONH2 (I) and not RC6H4CN:N(O)CONH2 (Bellavita, V.; Cagnoli, N.; 1939). Ii with CNn- gave the oximes (E)-RC6H4CH:NOH (II). IIi, and their (Z)-isomers, with ClO2SNCO, followed
by hydrolysi gave I. The configuration of I (R = 4-Br) was confirmed by x-ray anal. The monoclinic crystals, space group P21/c had a 14.39, b 5.101, c 12.5 Å, β 99.51°, Z = 4. The structure was
solved by Patterson and Fourier methods.

ACCESSION NUMBER: 1973:147493 CAPLUS
DOCUMENT NUMBER: 78:147493
TITLE: Unusual nitrones
AUTHOR(S): Dalton, D. R.; Foley, Henry G.; Trueblood, Kenneth N.;
Murphy, Michael R.
CORPORATE SOURCE: Dep. Chem., Temple Univ., Philadelphia, PA, USA
SOURCE: Tetrahedron Letters (1973), (10), 779-82
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **41514-44-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 41514-44-7 CAPLUS
CN Benzaldehyde, 3-nitro-, O-(aminocarbonyl)oxime, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L31 ANSWER 65 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN

GI For diagram(s), see printed CA Issue.

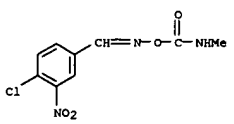
AB Thirty title compds. [I, R = Cl-4 alkyl, tetradecyl, MeOCH2, allyl, cyclohexyl, substituted phenyl; R1 = H, Me, or 4,3-Cl(O2N)C6H3; R2 = H, 2-Me, 2- or 4-Cl; R3 = 2, 3, or 4-NO2], used as selective herbicides in beet cultures, were prepared by reaction of oximes with isocyanates.
Thus,
m-O2NC6H4CH:NOH reacted with OCNMe in MeCN in the presence of Et3N at ≤30° to give 74.0% I (R = Me, R1 = R2 = H, R3 = 3-NO2) (II).
In postemergent tests 8 kg II/ha killed all Galinsoga parviflora or Urtica
urens without affecting beet plants.

ACCESSION NUMBER: 1973:29498 CAPLUS
DOCUMENT NUMBER: 78:29498
TITLE: Herbicidal nitrobenzaldoxime carbamates
INVENTOR(S): Stoelzer, Claus; Schmidt, Robert Rudolf
PATENT ASSIGNEE(S): Farbenfabriken Bayer A.-G.
SOURCE: Ger. Offen., 21 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

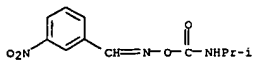
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2120087	A	19721109	DE 1971-2120087	19710424
PRIORITY APPLN. INFO.:			DE 1971-2120087 A	19710424

IT **39089-83-3P 39089-84-4P 39089-85-5P**
39089-86-6P 39089-87-7P 39089-88-8P
39089-89-9P 39089-90-2P 39089-91-3P
39089-94-6P 39089-95-7P 39089-96-8P
39089-97-9P 39089-98-0P 39089-99-1P
39090-00-1P 39090-01-2P 39090-02-3P
39090-04-5P 39090-06-7P 39102-00-6P
39102-01-7P 39102-02-8P 39102-03-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

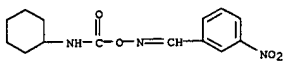
RN 39089-83-3 CAPLUS
CN Benzaldehyde, 4-chloro-3-nitro-, O-[(methylamino)carbonyl]oxime (9CI) (CA
INDEX NAME)



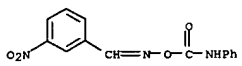
RN 39089-84-4 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[[(1-methylethyl)amino]carbonyl]oxime (9CI) (CA
INDEX NAME)



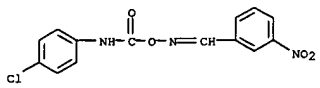
RN 39089-85-5 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[(cyclohexylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



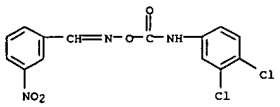
RN 39089-86-6 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[(phenylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



RN 39089-87-7 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[[(4-chlorophenyl)amino]carbonyl]oxime (9CI) (CA INDEX NAME)

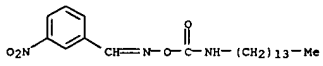


RN 39089-88-8 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[[(3,4-dichlorophenyl)amino]carbonyl]oxime (9CI) (CA INDEX NAME)

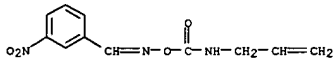


RN 39089-89-9 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[[(4-nitrophenyl)amino]carbonyl]oxime (9CI) (CA

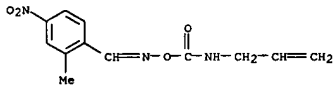
CN Benzaldehyde, 3-nitro-, O-[(tetradecylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



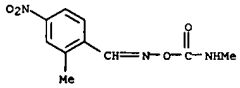
RN 39089-97-9 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[(2-propenylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



RN 39089-98-0 CAPLUS
CN Benzaldehyde, 2-methyl-4-nitro-, O-[(2-propenylamino)carbonyl]oxime (9CI) (CA INDEX NAME)

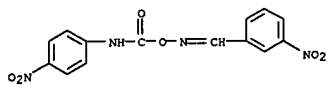


RN 39089-99-1 CAPLUS
CN Benzaldehyde, 2-methyl-4-nitro-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)

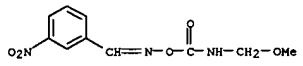


RN 39090-00-1 CAPLUS
CN Benzaldehyde, 4-chloro-2-nitro-, O-[[(1-methylethyl)amino]carbonyl]oxime (9CI) (CA INDEX NAME)

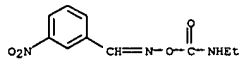
INDEX NAME)



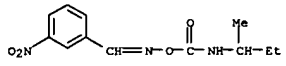
RN 39089-90-2 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[[(methoxymethyl)amino]carbonyl]oxime (9CI) (CA INDEX NAME)



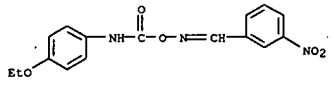
RN 39089-91-3 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[(ethylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



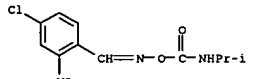
RN 39089-94-6 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[[(1-methylpropyl)amino]carbonyl]oxime (9CI) (CA INDEX NAME)



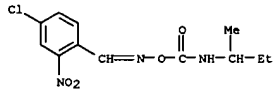
RN 39089-95-7 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[[(4-ethoxyphenyl)amino]carbonyl]oxime (9CI) (CA INDEX NAME)



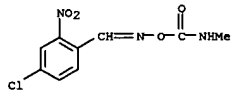
RN 39089-96-8 CAPLUS



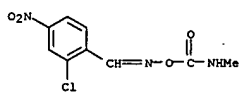
RN 39090-01-2 CAPLUS
CN Benzaldehyde, 4-chloro-2-nitro-, O-[[(1-methylpropyl)amino]carbonyl]oxime (9CI) (CA INDEX NAME)



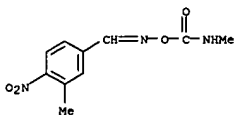
RN 39090-02-3 CAPLUS
CN Benzaldehyde, 4-chloro-2-nitro-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



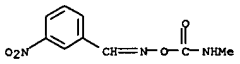
RN 39090-04-5 CAPLUS
CN Benzaldehyde, 2-chloro-4-nitro-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



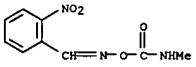
RN 39090-06-7 CAPLUS
CN Benzaldehyde, 3-methyl-4-nitro-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



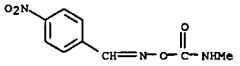
RN 39102-00-6 CAPLUS
CN Benzaldehyde, 3-nitro-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



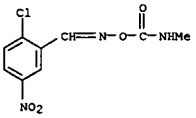
RN 39102-01-7 CAPLUS
CN Benzaldehyde, 2-nitro-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)



RN 39102-02-8 CAPLUS
CN Benzaldehyde, 4-nitro-, O-[(methylamino)carbonyl]oxime (9CI) (CA INDEX NAME)

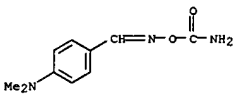


RN 39102-03-9 CAPLUS
CN Benzaldehyde, 2-chloro-5-nitro-, O-[(methylamino)carbonyl]oxime (9CI) (CA
INDEX NAME)



L31 ANSWER 66 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
GI For diagram(s), see printed CA Issue.
AB The oximes p-RC6H4CH:NOCONH2 (R = NMe2, Cl, OMe) were obtained in 55% yield by treating p-RC6H4CHO with NH2OH and KCNO. Hydrolysis of p-RC6-H4CH:NOCONH2 with KCN or Na2CO3 gave p-RC6H4CH:NOH. Treatment of p-ClC6H4CH:NOH with 2-tetrahydropyranyl isocyanate of ClSO2NCO gave I or p-ClC6H4CH:NOCONHSO2Cl, resp., both or which were hydrolized to p-ClC6H4CN.

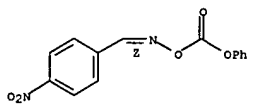
ACCESSION NUMBER: 1972:448002 CAPLUS
DOCUMENT NUMBER: 77:48002
TITLE: Hydroxylamine derivatives. 50. N-Carbamoyl oximes
AUTHOR(S): Zinner, Gerwalt; Ruthe, Helga
CORPORATE SOURCE: Inst. Pharm. Chem., Tech. Univ. Braunschweig, Brunswick, Fed. Rep. Ger.
SOURCE: Chemiker-Zeitung (1972), 96(5), 287-8
CODEN: CMKZAT; ISSN: 0009-2894
DOCUMENT TYPE: Journal
LANGUAGE: German
IT **38927-03-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 38927-03-6 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(aminocarbonyl)oxime (9CI) (CA INDEX NAME)



L31 ANSWER 67 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB A new synthesis of nitriles is reported based on the pyrolysis of oxime carbonates.

ACCESSION NUMBER: 1971:404873 CAPLUS
DOCUMENT NUMBER: 75:4873
TITLE: Pyrolysis of oxime carbonates: novel conversion of aldehydes into nitriles under mild conditions
AUTHOR(S): Prokipcak, Joseph M.; Forte, P. A.
CORPORATE SOURCE: Dep. Chem., Univ. Guelph, Guelph, ON, Can.
SOURCE: Canadian Journal of Chemistry (1971), 49(8), 1321-2
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 75:4873
IT **33620-19-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and pyrolysis of)
RN 33620-19-8 CAPLUS
CN Benzaldehyde, p-nitro-, O-carboxyoxime phenyl ester, (Z)- (8CI) (CA INDEX NAME)

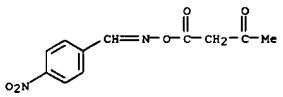
Double bond geometry as shown.



L31 ANSWER 68 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB The hydrolyses of carboxylic acid esters were studied kinetically to further establish the ElcB mechanism as an acyl transfer path for esters. The principal feature of this mechanism is elimination of the leaving group from the carbanion formed from the ester by ionization at a position α to the ester group. Such carbanion species were observed spectrophotometrically with all of the above esters and appeared during hydrolysis under conditions ranging from steady state through fast preequil. The nature of the leaving group has emerged as an extremely important factor in determining the relative contributions of the ElcB and BAc2 mechanisms. Yields of acetoacetanilide obtained from hydrolysis of p-nitrophenyl acetoacetate in the presence of aniline buffers have been examined in detail and compared with the kinetics of p-nitrophenol release. These results as well as those establishing a change of rate-limiting step with increase in general base concentration and the D solvent isotope effect are fully in accord with an ElcB hydrolysis mechanism which proceeds by way of a transient free ketene after elimination of the leaving group from the carbanion.

ACCESSION NUMBER: 1970:519837 CAPLUS
DOCUMENT NUMBER: 73:119837
TITLE: The carbanion mechanism (ElcB) of ester hydrolysis. III. Some structure-reactivity studies and the ketene intermediate
AUTHOR(S): Pratt, R. F.; Bruice, Thomas C.
CORPORATE SOURCE: Dep. of Chem., Univ. of California, Santa Barbara, CA, USA
SOURCE: Journal of the American Chemical Society (1970), 92(20), 5956-64
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **29817-01-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of, mechanism of)
RN 29817-01-4 CAPLUS
CN Benzaldehyde, p-nitro-, O-acetoacetyloxime (8CI) (CA INDEX NAME)

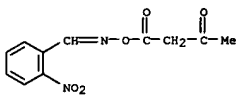


L31 ANSWER 69 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB The subject compds., prepared by the reaction of an aldoxime or ketoxime with diketene, show bactericidal activity. Thus, 36.6 g of a 55% solution of diketene in Me2CO is added to 8.8 g (CH:NOH)2 in 143 g Et2O containing 0.2 g triethylenediamine over 1 hr at 25-35°. After 2 hr the mixture is extracted with 5% aqueous Na2CO3 to yield 20.2 g bis(O-acetoacetyl)glyoxime, m. 128-30° (cyclohexane). The O-(acetoacetyl)oximes of the following carbonyl compds. are similarly prepared (m.p. and yield in g given): Ph-CHO (I), 60-1°, 63.4; 3,4-ClC6H3CHO (II), 84-6°, 40.1; 2-O2NC6H4CHO 63-6°, 11.1; Ph2CO, 68-70°, 16.2; 3-chloro-7-cyanonorbornan-2-one, 87-9°, 12.3. I gives partial and II gives complete control of Staphylococcus aureus, Escherichia coli, Erwinia amylovora, and Xanthomonas malvacearum at 250 ppm in potato dextrose agar culture tests.

ACCESSION NUMBER: 1970:43163 CAPLUS
DOCUMENT NUMBER: 72:43163
TITLE: O-Acetoacetyl oximes
INVENTOR(S): Marcus, Erich; Hughes, John L.
PATENT ASSIGNEE(S): Union Carbide Corp.
SOURCE: U.S., 5 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3483231	A	19691209	US 1966-529217	19660223
PRIORITY APPLN. INFO.:			US 1966-529217 A	19660223

IT **14146-72-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 14146-72-6 CAPLUS
CN Benzaldehyde, o-nitro-, O-acetoacetyloxime (8CI) (CA INDEX NAME)



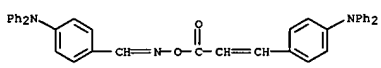
L31 ANSWER 70 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB Title compds. are useful photoconductors in production of electrophotographic recording materials. Thus, to a solution of 50 g 4-acetyltriphenyl-amine in tetrahydrofuran 3 equivalent aqueous KClO2 was added under stirring. After 2 hr, concentrated HCl was added, the precipitate filtered, and recrystd. from EtOH to give 72% p-Ph2NC6H4R (I, R = CO2H), m. 202-4°. The following I were prepared (R and m.p. given): CO2Me, 88.5-9.5°; C 6H2(CO2Et)Ph2-4,3,5, 64-6°; CH(OH)CH2C.tplbond.CH, ; CH2 oH, 93-4°; C2H4OH, 121°; CH(:NOH), 168-9°; CMe(:NOH), 140-1°; C6H12OH, (oil); C12H24OH, (oil); C2H4CO2H, 126-8°; CONPh2, ; OH, 126-8°; 2-OMe, 103-5°; 2-OH, 106-8°; CH(:NNHCONH2) 185-7°; CMe(:NNHCONH2), 177-8°. Also prepared were the following 4-Ph2NC6H4(CR1:CR2)nX (R1, R2, n, X, and m.p. given): H, H, 1, CO2H, 175.7-7.7°; H, H, 1, CO2Et, 70-2°; H, H, 1, COCl, 122-4°; H, H, 1, CONPh2, 201.5-3.5°; H, H, 1, CO(O)COCH:CHC6H4NPh2-4, 152-6°; Me, H, 1, CO2H, 191-2°; H, C(CO2H):CHC6H4NPh2-4, 1, CO2H, 211-14°; H, H, 1, H, (b0·12 138°); H, H, 1, CH(:NOH), 134-6°; H, H, 2, cO2H, 86-91°; H, H, 1, CO2N:CHC6H4NPh2-4, 174-8°; H, H, 1, CO2CH2C6H4NPh2, 68-70°; H, H, 2, CH(:NOH), ; H, H, 1, CO2Me, 108-9°. Also prepared was 1-(4-diphenylamino)-naphthacrylic acid, m. 247-8°, and 4-[N,N-bis(p-bromophenyl)-amino]cinnamic acid, m. 156-9°.

ACCESSION NUMBER: 1970:31416 CAPLUS
DOCUMENT NUMBER: 72:31416
TITLE: Substituted triarylamines with improved photoconductivity
INVENTOR(S): Brantly, Thomas B.; Fox, Charles J.
PATENT ASSIGNEE(S): Eastman Kodak Company
SOURCE: Ger. Offen., 34 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1908346	A	19691113	DE 1969-1908346	19690219
FR 2002221	A5	19691017	FR 1969-3822	19690217
BR 6906472	A0	19730118	BR 1969-206472	19690219
GB 1258094	A	19711222	GB 1969-1258094	19690220
PRIORITY APPLN. INFO.:			US 1968-706799 A	19680220
			US 1968-706780 A	19680220

IT **25069-78-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 25069-78-7 CAPLUS
CN Benzaldehyde, p-(diphenylamino)-, O-[p-(diphenylamino)cinnamoyl]oxime (8CI) (CA INDEX NAME)

L31 ANSWER 70 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L31 ANSWER 71 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN

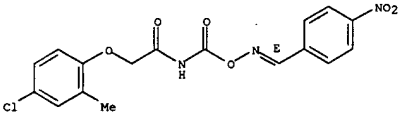
AB The title reaction proceeds vigorously at room temperature Aliphatic aldoximes, such as MeCH:NOH, give with RCONCO (I) (R is CH2F, CH2Cl, Et, PhOCH2, o-MeC6H4OCH2, o,p-Cl2C6H3OCH2, p-O2NC6H4OCH2, Ph, p-ClC6H4, or p-O2NC6H4) at room temperature only the corresponding RCONH2, MeCN, and CO2. The products of the aromatic aldoximes R1CH:NOH with I are RCONHCO2N:CHR1 (II) (R and R1 given): CH2F, Ph; CH2Cl, Ph; Et, Ph; PhOCH2, Ph; o-MeC6H4OCH2, Ph; o,p-Me-ClC6H3OCH2, Ph; o,p-MeClC6H3OCH2, Ph; o,p-Cl2C6H3OCH2, Ph; p-O2NC6H4OCH2, Ph; Ph, Ph; p-ClC6H4, Ph; p-O2NC6H4, Ph; p-O2NC6H4, p-O2NC6H4; o,p-Cl2C6H4, p-O2NC5H4; p-O2-NC6H4OCH2, p-Me2NC6H4; p-O2NC6H4, p-Me2NC6H4. However, at -5° to 0°, MeCH:NOH reacted with I (R = o,p-Me-ClC6H3OCH2) to give 70% II (R = o,p-MeClC6H3OCH2, R1 = Me). The reaction at room temperature gave only o,p-MeClC6H3-OCH2CONH2, MeCN, and CO2. The hydrolysis of II with NaOH gave RCO2H and R1CH:NOH, which proves that stable II exist only in syn configuration.

ACCESSION NUMBER: 1969:438478 CAPLUS
DOCUMENT NUMBER: 71:38478
TITLE: Acylisocyanates and their derivatives. III. Reaction of aldoximes with acyl isocyanates
AUTHOR(S): Nuridzhanyan, K. A.; Nesterova, L. M.; Vasil'ev, A. F.; Negrebetskii, V. V.
CORPORATE SOURCE: Vses. Nauch.-Issled. Inst. Khim. Sredstv Zashchity Rast., Moscow, USSR
SOURCE: Zhurnal Organicheskoi Khimii (1969), 5(5), 869-74
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian

IT **22998-04-5P 22998-05-6P 22998-06-7P 22998-07-8P 22998-08-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 22998-04-5 CAPLUS
CN Benzaldehyde, p-nitro-, O-[[[(4-chloro-o-tolyl)oxy]acetyl]carbamoyl]oxime, (E)- (8CI) (CA INDEX NAME)

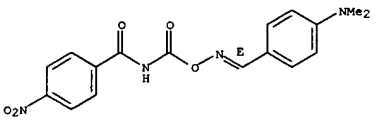
Double bond geometry as shown.



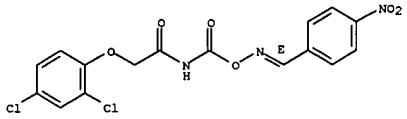
RN 22998-05-6 CAPLUS
CN Benzaldehyde, p-nitro-, O-[[(2,4-dichlorophenoxy)acetyl]carbamoyl]oxime, (E)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.

L31 ANSWER 71 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

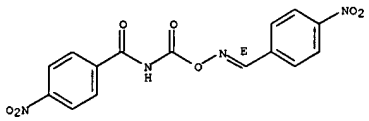


L31 ANSWER 71 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



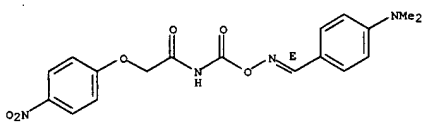
RN 22998-06-7 CAPLUS
CN Benzaldehyde, p-nitro-, O-[(p-nitrobenzoyl)carbamoyl]oxime, (E)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 22998-07-8 CAPLUS
CN Benzaldehyde, p-(dimethylamino)-, O-[[(p-nitrophenoxy)acetyl]carbamoyl]oxime, (E)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 22998-08-9 CAPLUS
CN Benzaldehyde, p-(dimethylamino)-, O-[(p-nitrobenzoyl)carbamoyl]oxime, (E)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.

L31 ANSWER 72 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN

AB The title compds. useful as insecticides, animal systemic parasiticides, herbicides, and foliage fungicides have the formula I. The intermediate 3-(diethoxyphosphinothioyl) benzaldehyde (II), n30D 1.5239 was prepared in 99.5% yield by refluxing 24.4 g. 3-hydroxybenzaldehyde, 37.8 g. O,O-diethylphos-phorochloridothioate, and 16.4 g. K2CO3 in 200 ml. Me Et ketone 4 hrs., the mixture poured into 300 ml. H2O and twice extracted with CHCl3, 7.5 g. Na2CO3.H2O added to a mixture of 27.4 g. II and 7.6 g. hydroxylamine hydrochloride in 300 ml. H2O at room temperature in 20 min., and the mixture stirred one hr. and extracted with C6H6 to give 68.3% 3-(diethoxyphosphinothioyl)benzaldoxime (III), n30D 1.5460. III (10 g.) in 10 ml. acetone was treated with excess MeNCO and poured into 200 ml. C6H6 to give 93.3% 3-(dieth-oxyphosphinothioyl) benzaldoxime methylcarbamate, n30D 1.5394. Similarly prepared in 96.9% yield was 4'-(diethoxyphosphino-thioyl)acetophenone oxime methylcarbamate. A mixture of 56.2 g. 4'-(diethoxyphosphinothioyl)acetophenone, 17.4 g. hydroxylamine hydrochloride, and 4 g. NaOH in 150 ml. 80% EtOH was refluxed 5 min., cooled, and acidified with concentrated HCl to give 93.5% 4'-(diethoxyphosphinothioyl)acetophenone oxime (IV), n30D 1.5393. A mixture of 10.0 g. IV, 3.2 g. AcCl, 4.1 g. Et3N, and 150 ml. C6H6 was refluxed one hr. to give 96.5% 4'-(diethoxy-phosphinothioyl)acetophenone oxime acetate, n30D 1.5279. A solution of 14.5 g. 4-(diethoxyphosphinothioyl)benzaldoxime. (V) in 50 ml. Et2O was added in 30 min. at 10° to 7 g. phosgene in 150 ml. Et2O, the mixture stirred one hr. at 15°, a solution of 17.4 g. morpholine in 10 ml. H2O added at <15°, and the mixture stirred two hrs. at room temperature and worked up to give 89.8% 4-(diethoxy-phosphinothioyl)benzaldoxime 4-morpholinecarboxylate, n30D 1.5423. Similarly 14.5 g. V, 7 g. phosgene, and 8.6 g. N,N-dimethylaniline treated with 6.1 g. ethanolamine and 10 ml. H2O at <15° gave 94.8% 4-(diethoxyphosphinothioyl)benzaldoxime (β-hydroxyethyl)carbamate (VI), n30D 1.5423. A solution of 11.6 g. N,N-diethylethylenediamine in 10 ml. H2O was added dropwise at <15° to VI in Et2O solution to give 51.8% 4-(diethoxyphos-phinothioyl)benzaldoxime 2-(diethylamino)ethyl carbamate, n30D 1.5310. These procedures were followed to obtain the tabulated I (X = S, p = position of phenyl substitution by R2C:NOR3 relative to P-containing group). The following VII were likewise prepared (R, R1, and n30D given): H, CONHMe, 1.5280; H, CONHBu, 1.5130; Me, CONHMe, 1.5243; Me, CONHPr-iso, 1.5109. The compds. prepared were tested as pre- and postemergent herbicides, as foliage fungicides, as insecticides, and for internal animal systematic activity.

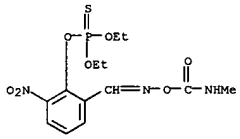
ACCESSION NUMBER: 1969:430236 CAPLUS
DOCUMENT NUMBER: 71:30236
TITLE: (O-Carbamoyl oxime), phosphate, phosphonate, and phosphinate compositions and their utility as herbicides and pesticides
INVENTOR(S): Gutman, Arnold D.
PATENT ASSIGNEE(S): Stauffer Chemical Co.
SOURCE: S. African, 80 pp.
CODEN: SFXXAB

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

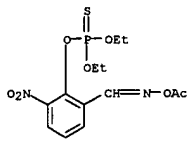
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ZA 6803662		19681108		
DE 1768676			DE	
FR 1583911			FR	
GB 1229853			GB	
US 3652737		19720000	US	
US 3673181		19720000	US	
US 3681476		19720000	US	
US 3681478		19720000	US	
US 3681479		19720000	US	
US 3733375		19730000	US	
US 3749748		19730000	US	
US 3769419		19730000	US	
PRIORITY APPLN. INFO.:			US	19670616
			US	19680520

IT **22936-26-1P 22936-27-2P 22936-28-3P 22936-40-9P 22936-41-0P 22939-83-9P 22939-85-1P 22939-86-2P 23107-33-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

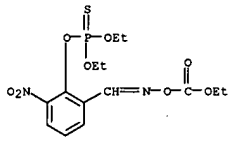
RN 22936-26-1 CAPLUS
CN Phosphorothioic acid, O,O-diethyl ester, O-ester with 3-nitrosalicylaldehyde O-(methylcarbamoyl)oxime (8CI) (CA INDEX NAME)



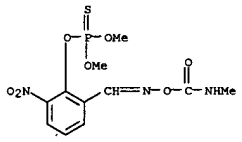
RN 22936-27-2 CAPLUS
CN Phosphorothioic acid, O,O-diethyl ester, O-ester with 3-nitrosalicylaldehyde O-acetyloxime (8CI) (CA INDEX NAME)



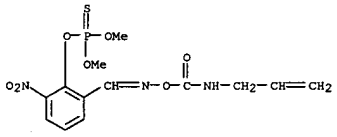
RN 22936-28-3 CAPLUS
CN Phosphorothioic acid, O,O-diethyl ester, O-ester with 3-nitrosalicylaldehyde O-(ethoxycarbonyl)oxime (8CI) (CA INDEX NAME)



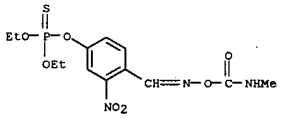
RN 22936-40-9 CAPLUS
CN Phosphorothioic acid, O,O-dimethyl ester, O-ester with 3-nitrosalicylaldehyde O-(methylcarbamoyl)oxime (8CI) (CA INDEX NAME)



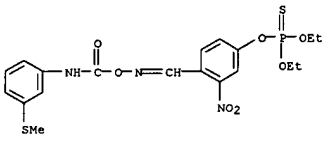
RN 22936-41-0 CAPLUS
CN Phosphorothioic acid, O,O-dimethyl ester, O-ester with 3-nitrosalicylaldehyde O-(allylcarbamoyl)oxime (8CI) (CA INDEX NAME)



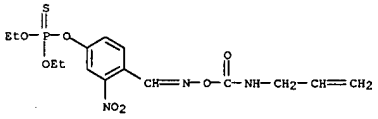
RN 22939-83-9 CAPLUS
CN Phosphorothioic acid, O,O-diethyl ester, O-ester with 4-hydroxy-2-nitrobenzaldehyde O-(methylcarbamoyl)oxime (8CI) (CA INDEX NAME)



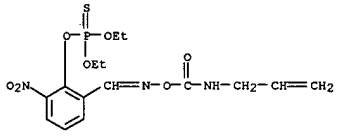
RN 22939-85-1 CAPLUS
CN Phosphorothioic acid, O,O-diethyl ester, O-ester with 4-hydroxy-2-nitrobenzaldehyde O-[[m-(methylthio)phenyl]carbamoyl]oxime (8CI) (CA INDEX NAME)



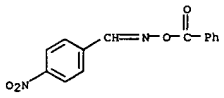
RN 22939-86-2 CAPLUS
CN Phosphorothioic acid, O,O-diethyl ester, O-ester with 4-hydroxy-2-nitrobenzaldehyde O-(allylcarbamoyl)oxime (8CI) (CA INDEX NAME)



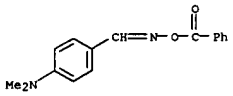
RN 23107-33-7 CAPLUS
CN Phosphorothioic acid, O,O-diethyl ester, O-ester with 3-nitrosalicylaldehyde O-(allylcarbamoyl)oxime (8CI) (CA INDEX NAME)



L31 ANSWER 73 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB The pyrolytic elimination of BzOH from 8 substituted benzoyl-α-benzaldoximes to yield the corresponding substituted benzonitriles shows first-order kinetics in 5 solvents. The plot of log k vs. σ is linear for this reaction in the solvents Tetralin, o-di-chlorobenzene, Me2SO, and AcNHMe, but not HCONMe2, in which competing base catalysis by the solvent occurs. Thermodynamic parameters and small neg. values for ρ indicate that the reaction mechanism is essentially synchronous. Catalysis by a wide range of metal salts was observed. 26 references.
ACCESSION NUMBER: 1968:29150 CAPLUS
DOCUMENT NUMBER: 68:29150
TITLE: Pyrolysis of benzoyl-α-benzaldoximes. I. Effect of substitution, solvents, and catalysts
AUTHOR(S): Hill, John H. M.; Schmookler, Linda D.
CORPORATE SOURCE: Hobart and William Smith Colleges, Geneva, NY, USA
SOURCE: Journal of Organic Chemistry (1967), 32(12), 4025-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **3848-35-9 4058-69-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(pyrolysis of, solvent and substituent effects in)
RN 3848-35-9 CAPLUS
CN Benzaldehyde, 4-nitro-, O-benzoyloxime (9CI) (CA INDEX NAME)

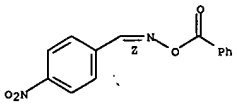


RN 4058-69-9 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-benzoyloxime (9CI) (CA INDEX NAME)

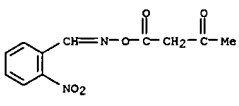


L31 ANSWER 74 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
GI For diagram(s), see printed CA Issue.
AB cf. CA 63: 7904d. Dipole moments of oxime O-acyl derivs. I-VII were measured in C6H6 or dioxane solution and configurations and conformations were determined by means of the previously described graphical method. In all derivs. the acyl group has a stable conformation s-trans as in esters and other similar compds. In benzoyl derivs. of benzaldoximes the double bond C:N has a stable configuration syn.
ACCESSION NUMBER: 1967:463622 CAPLUS
DOCUMENT NUMBER: 67:63622
TITLE: Oxime derivatives. IX. Determination of configuration and conformation of acylated oximes on the basis of dipole moments
AUTHOR(S): Exner, Otto; Hollerova, J.; Jehlicka, Vladimir
CORPORATE SOURCE: Ust. Fys. Chem., Vys. Skola Chem. Technol., Prague, Czech.
SOURCE: Collection of Czechoslovak Chemical Communications (1967), 32(6), 2096-103
CODEN: CCCCAK; ISSN: 0010-0765
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **18322-89-9**
RL: PRP (Properties)
(stereochemistry of)
RN 18322-89-9 CAPLUS
CN Benzaldehyde, 4-nitro-, O-benzoyloxime, [C(Z)]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L31 ANSWER 75 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
GI For diagram(s), see printed CA Issue.
AB The reaction of diketene with oximes in the presence of 1,4-diazabicyclo[2.2.2]octane gave good yields of new derivs., of oximes, the O-acetoacetyl derivs. Attempted O-acetoacetylation of N-phenylpyruvamidoxime led to 4-acetyl-3-methyl-1-phenyl-3-pyrroline-2,5-dione 2-oxime (I) and the O-acetoacetylation of the oxime of dehydroacetic acid gave 3,6-dimethyl-4H-pyrano [3,4-d]isoxazol-4-one.
ACCESSION NUMBER: 1967:54976 CAPLUS
DOCUMENT NUMBER: 66:54976
TITLE: Reactions of oximes with diketene
AUTHOR(S): Marcus, Erich; Chan, John K.; Hughes, John Lawrence
CORPORATE SOURCE: Chem. Div., Union Carbide Corp., South Charleston, WV, USA
SOURCE: Journal of Chemical and Engineering Data (1967), 12(1), 151-3
CODEN: JCEAAX; ISSN: 0021-9568
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **14146-72-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 14146-72-6 CAPLUS
CN Benzaldehyde, o-nitro-, O-acetoacetyloxime (8CI) (CA INDEX NAME)



L31 ANSWER 76 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB cf. CA 59, 5167g. RC(NH2):NO2CR' (I) and RCH:NO2CR' (II) are considered to be activated esters and can be used as acylating agents. Some I and II were compared in their reaction with PhCH2NH2 (III). The kinetic consts., k (min.-1), of the reaction of 0.05M p-MeOC6H4CH:NO2CC6H4NO2-p, p-O2NC6H4CO2N:CHPh, and p-O2NC6H4CO2N:CHC6H4NO2-p with 0.1M III in 1:1 dioxane-HCONMe2 at 25° were found to be 2.7 + 10-3, 4.0 + 10-3, and 2.3 + 10-2, resp.; k of the reaction of 0.05M p-O2NC6H4C(NH2):NOAc, PhC(NH2):NOAc, p-MeOC6H4C(NH2):NOAc, and PhC(NEt2):NOAc and 0.1M III in dioxane at 25° were found to be 4.9 + 10-3, 2.9 + 10-3, 1.4 + 10-3, and 4.4 + 10-4, resp.; k of 0.05M RCO2R' (IV) and 0.1M III at 25° were for IV (R = Me) in dioxane: R' = p-O2NC6H4, 3.0 + 10-2; R' = PhC(NH2):N, 2.9 + 10-3; R' = NCCH2, 1.7 + 10-4; R' = Et, .apprx.10-6; for IV((R = Ph) [all in 1:1 dioxane-HCONMe2]: R' = p-O2NC6H4, 3 + 10-1; R' = PhC(NH2):N, 3.0 + 10-5; R' = NCCH2, 3.8 + 10-5; for IV (R = p-O2NC6H4): R' = p-O2NC6H4, .apprx.10; R' = PhC(NH2):N, 4.3 + 10-4; R' = NCCH2, 5.9 + 10-4; R' = Et, .apprx.10-7; for IV [R = 2-(5-nitrofuryl)]: R' = p-O2NC6H4, ∞; R' = PhC(NH2):N, 4.7 + 10-3; R' = NCCH2, 2.1 + 10-2; R' = Et, 7 + 10-5. Dropwise addition of 7.75 g. PhCCl:NOH in 50 ml. Et2O to 7.3 g. Et2NH in 100 ml. Et2O gave PhC(NEt)2:NOH, m. 81° (petr. ether). Dropwise addition of 0.01 mole R'COCl in 25 ml. tetrahydrofuran (THF) to 0.02 mole RC(NH2):NOH in 50 ml. THF gave 100% I, of which the following were prepared (R, R', and m.p. given): p-MeOC6H4, Me, 102° (EtOAc-C6H14); Ph, p-O2NC6H4, 220° (HCONMe2-EtOH); Ph, 2-(5-nitrofuryl), 218° (EtOAc). PhC(NEt2):NOAc b0.01118°. Refluxing 0.02 mole the appropriate oxime and 0.02 mole p-O2NC6H4COCl in 100 ml. Et2O 3 hrs. gave 100% the following p-O2NC6H4CO2N:CHR (R' and m.p. or b.p. given): p-MeOC6H4, 171° (HCONMe2-EtOH); p-O2NC6H4, 197° (HCONMe2-EtOH); Me, b25 78°; and 70-95% of the following NCCH2CO2R (same data): Ph, b0.6 91°; p-O2NC6H4, 85° (Et2O); 2-(5-nitrofuryl), 122° (EtOAc-C6H14). Dropwise addition of 0.02 mole 2-(5-nitrofuroyl) chloride in 20 ml. Et2O to 0.02 mole p-O2NC6H4OH and 0.02 mole C5H5N in 50 ml. Et2O gave 100% p-nitrophenyl 5-nitrofuroate, m. 193° (HCONMe2-EtOH). The acylating power of I and II is directly related to the acidity of the OH of the alc. or oxime.
ACCESSION NUMBER: 1965:29263 CAPLUS
DOCUMENT NUMBER: 62:29263
ORIGINAL REFERENCE NO.: 62:5157g-h,5158a-e
TITLE: Activated esters. I. Aminolysis of acylated oxime and amidoxime derivatives
AUTHOR(S): Buyle, R.
CORPORATE SOURCE: Union Carbide European Res. Assocs., Brussels, Belg.
SOURCE: Helvetica Chimica Acta (1964), 47(8), 2444-8
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: French
IT **1044-74-2**, Benzaldehyde, p-nitro-, O-(p-nitrobenzoyl)oxime
(reaction with benzylamine)
RN 1044-74-2 CAPLUS
CN Benzaldehyde, 4-nitro-, O-(4-nitrobenzoyl)oxime (9CI) (CA INDEX NAME)

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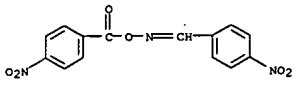
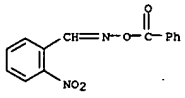
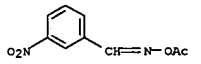


L31 ANSWER 77 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB Refluxing p-anisidine and bis(p-nitrophenyl) carbonate (I) in dioxane 1 hr., followed by dilution with H2O and 10 hrs. at room temperature, gave 39%
p-O2NC6H4O2CNRR' (II) (R, R', and m.p. given): H, p-MeOC6H4, 133-5°; iso-Bu, H, 110° (87%); p-ClC6H4, H, 161-3° (99%); p-MeC6H4, H, 114.5-15.5° (63%); p-HO2CC6H4, H, 179.5-80° (86%); 2-pyridyl,.H, 116° (46%). I and Et2NH heated 1 hr. on a steam bath gave 75% II (R = R' = Et), b746 280-2° (decomposition); PhNHEt and I in 2 hrs. at 150° gave 52% II (R = Ph, R' = Et), m. 76°; Ph2NH and I gave 19% II (R = R' = Ph), m. 139-40°. I and o-HO C6H4NH2 in 3 hrs. at 100° gave 46% II (R = o-HOC6H4, R' = H), m. 110-11°.
ACCESSION NUMBER: 1965:15144 CAPLUS
DOCUMENT NUMBER: 62:15144
ORIGINAL REFERENCE NO.: 62:2725e-f
TITLE: Synthesis of p-nitrophenyl esters of substituted carbamic acids
AUTHOR(S): Nesynov, E. P.; Pel'kis, P. S.
CORPORATE SOURCE: Inst. Org. Chem., Kiev
SOURCE: Zhurnal Obshchei Khimii (1964), 34(10), 3467-9
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT **3848-29-1**, Benzaldehyde, o-nitro-, O-benzoyloxime
3848-31-5, Benzaldehyde, m-nitro-, O-acetyloxime **3848-32-6**, Benzaldehyde, m-nitro-, O-benzoyloxime **3848-34-8**, Benzaldehyde, p-nitro-, O-acetyloxime **3848-35-9**, Benzaldehyde, p-nitro-, O-benzoyloxime **3986-36-5**, Benzaldehyde, p-(dimethylamino)-, O-acetyloxime **4058-69-9**, Benzaldehyde, p-(dimethylamino)-, O-benzoyloxime
(preparation of)
RN 3848-29-1 CAPLUS
CN Benzaldehyde, o-nitro-, O-benzoyloxime (7CI, 8CI) (CA INDEX NAME)

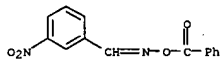


RN 3848-31-5 CAPLUS
CN Benzaldehyde, m-nitro-, O-acetyloxime (7CI, 8CI) (CA INDEX NAME)

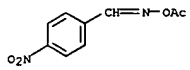


RN 3848-32-6 CAPLUS
CN Benzaldehyde, m-nitro-, O-benzoyloxime (7CI, 8CI) (CA INDEX NAME)

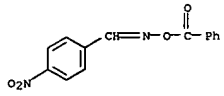
L31 ANSWER 77 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



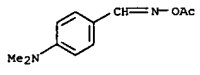
RN 3848-34-8 CAPLUS
CN Benzaldehyde, p-nitro-, O-acetyloxime (7CI, 8CI) (CA INDEX NAME)



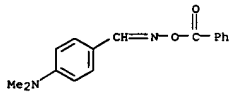
RN 3848-35-9 CAPLUS
CN Benzaldehyde, 4-nitro-, O-benzoyloxime (9CI) (CA INDEX NAME)



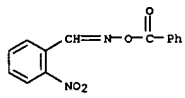
RN 3986-36-5 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-acetyloxime (9CI) (CA INDEX NAME)



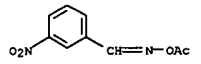
RN 4058-69-9 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-benzoyloxime (9CI) (CA INDEX NAME)



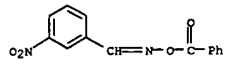
L31 ANSWER 78 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB Substances described as arylideneureas by Bellavita and Cagnoli (CA 34, 19782) were shown to be oximes of the corresponding aldehydes used for the
synthesis. This conclusion was verified by ir spectra.
ACCESSION NUMBER: 1965:15143 CAPLUS
DOCUMENT NUMBER: 62:15143
ORIGINAL REFERENCE NO.: 62:2725e
TITLE: Synthesis of arylideneureas
AUTHOR(S): Sedova, V. F.; Mamaev, V. P.
CORPORATE SOURCE: Inst. Org. Chem., Novosibirsk
SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1964), (10), 1892-3
CODEN: IASKA6; ISSN: 0002-3353
DOCUMENT TYPE: Journal
LANGUAGE: Russian
IT **3848-29-1**, Benzaldehyde, o-nitro-, O-benzoyloxime
3848-31-5, Benzaldehyde, m-nitro-, O-acetyloxime **3848-32-6**, Benzaldehyde, m-nitro-, O-benzoyloxime **3848-34-8**, Benzaldehyde, p-nitro-, O-acetyloxime **3848-35-9**, Benzaldehyde, p-nitro-, O-benzoyloxime **3986-36-5**, Benzaldehyde, p-(dimethylamino)-, O-acetyloxime **4058-69-9**, Benzaldehyde, p-(dimethylamino)-, O-benzoyloxime
(preparation of)
RN 3848-29-1 CAPLUS
CN Benzaldehyde, o-nitro-, O-benzoyloxime (7CI, 8CI) (CA INDEX NAME)



RN 3848-31-5 CAPLUS
CN Benzaldehyde, m-nitro-, O-acetyloxime (7CI, 8CI) (CA INDEX NAME)

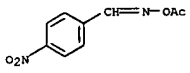


RN 3848-32-6 CAPLUS
CN Benzaldehyde, m-nitro-, O-benzoyloxime (7CI, 8CI) (CA INDEX NAME)

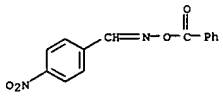


RN 3848-34-8 CAPLUS
CN Benzaldehyde, p-nitro-, O-acetyloxime (7CI, 8CI) (CA INDEX NAME)

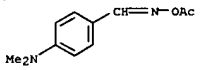
L31 ANSWER 78 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



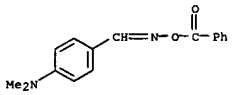
RN 3848-35-9 CAPLUS
CN Benzaldehyde, 4-nitro-, O-benzoyloxime (9CI) (CA INDEX NAME)



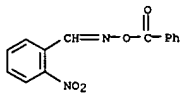
RN 3986-36-5 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-acetyloxime (9CI) (CA INDEX NAME)



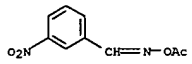
RN 4058-69-9 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-benzoyloxime (9CI) (CA INDEX NAME)



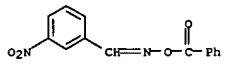
L31 ANSWER 79 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB RCONCS and Cl yield RCON:CCl2 or RCON:CClSCl depending on reactant ratio used. These react with amines, alcs., or phenols yielding the corresponding derivs. PhCON:CCl2, b12 124-6°, n20D 1.5670, d20 1.3345; o-ClC6H4CON:CCl2, b20 160-2°, 1.5824, 1.4511 (p-isomer b17 153-4°, 1.5900, 1.4344); PhCON:CClSCl, m. 91-2°; p-ClC6H4CON:CClSCl, m. 112-14°; PhCON:C(NHPh)SNHPh, m. 101-3°. No details are given.
ACCESSION NUMBER: 1965:15142 CAPLUS
DOCUMENT NUMBER: 62:15142
ORIGINAL REFERENCE NO.: 62:2725d-e
TITLE: N-Acyl isothiocyanate derivatives
AUTHOR(S): Ivanova, Zh. M.; Derkach, G. I.; Kirsanova, N. A.
CORPORATE SOURCE: Inst. Org. Chem., Kiev
SOURCE: Zhurnal Obshchei Khimii (1964), 34(10), 3516-18
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT **3848-29-1**, Benzaldehyde, o-nitro-, O-benzoyloxime
3848-31-5, Benzaldehyde, m-nitro-, O-acetyloxime **3848-32-6**, Benzaldehyde, m-nitro-, O-benzoyloxime **3848-34-8**, Benzaldehyde, p-nitro-, O-acetyloxime **3848-35-9**, Benzaldehyde, p-nitro-, O-benzoyloxime **3986-36-5**, Benzaldehyde, p-(dimethylamino)-, O-acetyloxime **4058-69-9**, Benzaldehyde, p-(dimethylamino)-, O-benzoyloxime
(preparation of)
RN 3848-29-1 CAPLUS
CN Benzaldehyde, o-nitro-, O-benzoyloxime (7CI, 8CI) (CA INDEX NAME)



RN 3848-31-5 CAPLUS
CN Benzaldehyde, m-nitro-, O-acetyloxime (7CI, 8CI) (CA INDEX NAME)

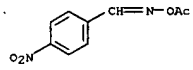


RN 3848-32-6 CAPLUS
CN Benzaldehyde, m-nitro-, O-benzoyloxime (7CI, 8CI) (CA INDEX NAME)

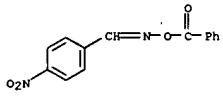


RN 3848-34-8 CAPLUS

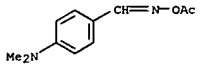
L31 ANSWER 79 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN Benzaldehyde, p-nitro-, O-acetyloxime (7CI, 8CI) (CA INDEX NAME)



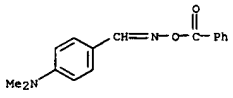
RN 3848-35-9 CAPLUS
CN Benzaldehyde, 4-nitro-, O-benzoyloxime (9CI) (CA INDEX NAME)



RN 3986-36-5 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-acetyloxime (9CI) (CA INDEX NAME)

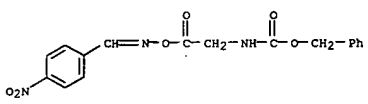


RN 4058-69-9 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-benzoyloxime (9CI) (CA INDEX NAME)

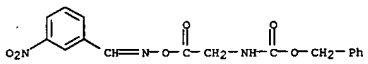


L31 ANSWER 80 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB (Cbo = PhCH2O2C throughout this abstract) Carbobenzoxyglycine (I) reacted with a series of oximes by the anhydride method (A) (Weygand and Steglich, CA 55, 5359b) (average yields 70%) and with Ph2C:CO (method B) (Elmore and Smyth, CA 59, 4033a) (unfavorable results) to give aminoacyl oximes, PhCH2O2CNHCH2CO2N:CRR1, (II), whose rates of aminolysis by PhCH2NH2 were determined in tetrahydrofuran (THF) at 22°. The results were plotted and discussed from the standpoint of substituent effects on carboxyl activation. The new activation method for peptide synthesis was tested with some simple examples. The following standards were prepared from comparative aminolysis: I thiophenyl ester, m. 72°, from I, PhSH, and POCl3 in absolute THF at -15°; I p-nitrophenyl ester, m. 131°. From I, p-O2NC6H4OH, and POCl3 in THF; and I benzyl ester, m. 71°, from equimolar amts. I and PhCH2Cl in boiling dioxane with excess Et3N. Method A. I (20 millimoles) and 20 millimoles absolute Et3N in 20-30 cc. THF treated with 20 millimoles ClCO2Et at -15° with stirring, after 30 min. a solution of the appropriate oxime in THF added, and the mixture stirred 12 hrs. at -15°, kept overnight at room temperature, and worked up (Wieland and Heinke, CA 53, 18880f) gave II. Method B. I (20 millimoles) in THF treated with 20 millimoles Ph2C:CO and 4 cc. M THF-absolute Et3N at -15°, followed after several min. by 20 millimoles appropriate oxime in THF, the solution warmed gradually to room temperature, kept overnight, and worked up, and the product recrystd. from EtOAc-petr. ether or Me2CO-petr. ether gave II. The following II were prepared (R, R1, and m.p. given): Me, Me (III), 110-12°; (RR' =) cyclohexylidene, 80.5-1.5°; H, m-O2NC6H4, 126.5-8.0°; H, p-O2NC6H4, 166.5-7.5°; Me, Ph, 95.5-7.0°; Me, p-tolyl, 104°; Me, p-anisyl, 90°; Ph, Ph (IV), 78-9°; H, α-C10H7 (V), 107-8°; Me, p-BrC6H4, 113-14°, and Me, m-O2NC6H4 (VI), 79-80°. To 10 millimoles I and 10 millimoles absolute Et3N in 30 cc. THF was added 10 millimoles ClCO2Et at -15° with stirring, after 30 min. 10 millimoles appropriate alc. [furfuryl alc., furfuryl mercaptan (VII), or 1-phenyl-3-methyl-5-pyrazolone (VIII)] added, the mixture kept 5 hrs. at room temperature and worked up, and the crude product recrystd. from EtOAc-petr. ether to give I furfuryl ester, m. 70-1°; carbobenzoxyglycyl ester of VII, m. 65-6°; and I 1-phenyl-3-methylpyrazolyl ester (IX) (VIII bound to I as enol ester according to the ir spectrum), m. 131°, resp. EtO2CCH2NH2·HCl (X.HCl) (10 millimoles) suspended in 20 cc. MeCN treated with 10 millimoles absolute Et3N, followed by 10 millimoles III in MeCN, and the mixture kept 24 hrs. at room temperature and worked up gave 61.2% Cbo-Gly-Gly-OEt (XI), m. 81-2°. Similar treatment of 10 millimoles X.HCl in MeCN with 10 millimoles VI, V, and IX gave XI, m. 81-2°, in yields of 73, 85, and 75%, resp. From 50-millimoles amts. L-tyrosine Et ester-HCl (XII.HCl), IV, and absolute Et3N in MeCN was similarly prepared 75% Cbo-Gly-Tyr-OEt (XIII), m. 126-7°, [α]22D 19.1° (c 3, EtOH), and from 50-millimole amts. XII.HCl and IX was similarly prepared 90% XIII, m. 126-7°, [α]22D 19.0° (c 3, EtOH).

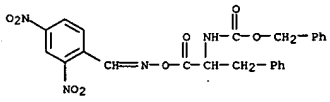
L31 ANSWER 80 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
ACCESSION NUMBER: 1965:3302 CAPLUS
DOCUMENT NUMBER: 62:3302
ORIGINAL REFERENCE NO.: 62:631f-h,632a-c
TITLE: N-Protected aminoacyl oximes as new carboxyl-activated compounds for peptide synthesis
AUTHOR(S): Losse, Guenter; Barth, Alfred; Schatz, Karin
CORPORATE SOURCE: Univ. Halle, Germany
SOURCE: Justus Liebigs Annalen der Chemie (1964), 677, 185-90
CODEN: JLACBF; ISSN: 0075-4617
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 62:3302
IT **3065-06-3**, Benzaldehyde, p-nitro-, O-[N-carboxyglycyl]oxime, benzyl ester **3065-07-4**, Benzaldehyde, m-nitro-, O-[N-carboxyglycyl]oxime, benzyl ester
(preparation of)
RN 3065-06-3 CAPLUS
CN Carbamic acid, [[[[(p-nitrobenzylidene)amino]oxy]carbonyl]methyl]-, benzyl ester (8CI) (CA INDEX NAME)



RN 3065-07-4 CAPLUS
CN Carbamic acid, [2-[[[(3-nitrophenyl)methylene]amino]oxy]-2-oxoethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



L31 ANSWER 81 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



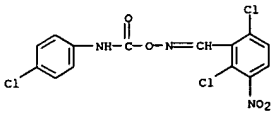
L31 ANSWER 81 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB The dissociation consts. (as pK) of several phenols, oximes, and hydroxamic acids was determined Many of these were condensed with benzyloxycarbonyl-L-phenylalanine (I) by the dicyclohexylcarbodiimide procedure. Then the rate of coupling of these esters was compared with an excess of PhCH2NH2 (II) in dioxane-water using as a measure of reactivity the first order half-reaction time (t/2) which was calculated from the change of the optical d. of the reaction mixture with time. Preparative scale reactions of phenolic esters of I with II and with H2NCH2CO2Et gave desired products in yields above 75%. Esters of slightly acidic phenols with I reacted slowly with amines, but 2,4,6-(O2N)3C6H2OH (pK 0.29) had such high reactivity with I that the ester could not be isolated but immediately disproportionated to the anhydride of I. The reactions of phenol esters of I with II were as follows [R of phenol HOR, pK, and t/2 (min.) given]: 4-Me2NC6H4, --, no reaction; 4-PhC6H4, 13.00, very slow; 4-FC6H4, 13.10, very slow; 4-ClC6H4, 12.51, 700; 2-FC6H4, 12.15, 555; 3-FC6H4, 12.42, 500; 3 ClC6H4, 12.09, 360; 2,4,6-I3C6H2, 8.24, 350; 2-ClC6H4, 11.98, 264; 3-pyridyl, 11.55, 172; 4-AcC6H4, 11.18, 157; N-methyl-3-pyridinium group 6.75, ?; 3,5-Cl2C6H3, 10.70, 44.4; 4-EtO2CC6H4, 11.35, 42.1; 2,4-Cl2C6H3, 10.87, 38.5; 2,4-MeO(OHC)C6H3, 10.30, 31.0; 2,4-Br2C6H3, 10.82, 31.0; 2,4,6-Cl3C6H2, 9.69, 19.3; 2,4-6-Br3C6H2, 8.29, 72.0; 4-O2NC6H4, 9.41, 5.7; 4-ONC6H4, 8.22, 4.3; 2,4,5-Cl3C6H2 9.60, 2.8; Cl5C, 6.25, 2.36. The hydroxamic acid or aldoxime, its pK, and the % yield from the reaction of its derivative of I with II were as follows: HONHCO2CH2Ph, 14.3, 68; HONHSO2Ph, 13.1, 78; BzNHOH (III), 11.4, 72; 4-O2NC6H4NHOH, 9.9, 85; AcNHOH, 14.5, 60; HON:CHPh, 14.5, 90; 2,4-(O2N)2C6H3CH:NOH, 12.0, 92; 3-HON:CHQ (Q = pyridyl), 13.4, 83; 4-HON:CHQ, 13.1, 84; HONHCOCH2Cl, 10.8, side reaction; HON:C(NH2)CH2Cl, 8.8, side reaction; HON:C(NH2)CCl3, strongly acid, side reaction. The t/2 of the reaction of the mixed anhydride of I and III with II was 44 min.
ACCESSION NUMBER: 1965:3293 CAPLUS
DOCUMENT NUMBER: 62:3293
ORIGINAL REFERENCE NO.: 62:627g-h,628g-h,629a
TITLE: Use of some new active esters in peptide synthesis
AUTHOR(S): Pless, J.
CORPORATE SOURCE: Sandoz Ltd., Basel, Switz.
SOURCE: Peptides, Proc. European Symp., 5th, Oxford (1963), 1962, 69-72
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **3267-57-0**, Carbamic acid, [α-[[[(2,4-dinitrobenzylidene)amino]oxy]carbonyl]phenethyl]-, benzyl ester
(reaction with benzylamine)
RN 3267-57-0 CAPLUS
CN Carbamic acid, [α-[[[(2,4-dinitrobenzylidene)amino]oxy]carbonyl]phenethyl]-, benzyl ester (7CI, 8CI) (CA INDEX NAME)

L31 ANSWER 82 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB The title compds. were prepared by chlorinating benzaldoximes in the presence of diluents with suitable isocyanates. The compds. exhibited usefulness as pre- and postemergent weed killers, in most cases more effective than Me2C:NO2CNHPh. Thus, 12.5 g. PhNCO added dropwise at 60° to a solution of 2,6-Cl2C6H3CH:NOH in 200 ml. absolute C6H6 and the mixture refluxed 30 min. gave 23 g. 2,6-Cl2C6H3CH:NO2CXHPh, m. 112-13° (decomposition). Similarly were obtained the following 2,6-Cl2C6H3CH:NO2CNHR [R and m.p. (decomposition) given]: 4-ClC6H4, 108-13°; 3-ClC6H4, 129-31°; 3,4-Cl2C6H3, 156°; 4-O2NC6H4, 144°; 4-EtOC6H4, 109-12°; 1-naphthyl, 180°; 1,2,3,4,5Cl5C2, 150°. 2,6-Cl2C6H3CH:NO2CNHSO2C6H4Me-4 m. 117-18° (decomposition). 2,6-Cl2C6H3CH:NOH (38 g.) in 200 ml. CH2Cl2 treated dropwise at 20-5° with 1,2,6-Me(OCN)2C6H3 in 100 ml. CH2Cl2 and the mixture stirred 6 hrs. at room temperature gave 31 g. (2,6-Cl2C6H3CH:NO2CNH)2R (I, R = 1-methyl-2,6-phenylene), m. 195° (decomposition). Similarly were prepared the following I (R and m.p. given): 1-methyl-2,4-phenylene, 147° (decomposition); 1,4-phenylene, <140° (decomposition); (4-C6H4)2CH2, <90°; 1,5naphthylene, <200° (decomposition); 1,4-cyclohexylene, 132-5°; (4-C6H4)2CMe2, 145° (decomposition); 1,3-phenylene, <130° (de-composition); 1,3,4-trichloro-5-methyl-2,6-phenylene, 180° (de-composition); 4,4'-dicyclohexylenemethyl, 130° (decomposition). 2,6-Cl2C6H3CH:NOH (28.5 g.) in 200 ml. CH2Cl2 treated dropwise at 20-5° with 23.3 g. (4-OCNC6H4O)3PS in CH2Cl2 and the mixture stirred 7 hrs. at room temperature, gave 50 g. [4-(2,6-Cl2C6H3CH:NO2CNH)C6H4O]3P(S), m. 90-100° (decomposition). 2,3,6-Cl3C6H2CH:NOH (45 g.) in 200 ml. CH2Cl2 treated dropwise at 20° with 24 g. PhNCO and the solution kept 3 hrs. gave 56 g. 2,3,6-Cl3C6H2CH:NO2CNHR (II, R = Ph), m. 55-60° (decomposition). Similarly were prepared the following II [R and m.p. (decomposition) given]: 3-ClC6H4, 98°; 4-ClC6H4, 94°; 3,4-Cl2C6H3, 118-20°; 1,2,3,4,5-Cl5C, 161°. 2,3,6-Cl3C6H2CH:NO2CNHSO2C6H4Me-4 137-9° (decomposition). 2,3,6-Cl3C6H1:NOH (45 g.) in 200 ml. CH2Cl2 treated dropwise at 20° with 14.7 g. 1,2,4-Me(OCN)2C6H3 and the mixture stirred 4 hrs. gave 58 g. 2,4-(2,3,6-Cl3C6H2CH:NO2CNH)2C6H3Me m. 210° (decomposition). 2,6,3-Cl2(O2N)C6H2:NOH (47 g.) in 200 ml. Et2O treated dropwise at 20° with 30.7 g. p-ClC6H4NCO in Et2O gave 60 g. 2,6,3-Cl2(O2N)C6H2CH:NO2CNHR (III, R = 4-ClC6H4), m. 158-64° (decomposition). Similarly prepared were the following III [R and m.p. (decomposition) given]: 3-ClC6H4, 128°; 3,4-Cl2C6H3, 147°. 2,6,3-Cl2(O2N)C6H2CH:NO2CNHSO2C6H4Me-4, m. 140-1°. 2,6,3-Cl2(MeO)C6H2:NOH (11 g.) in 300 ml. CH2Cl2 treated at 35-40° with 6 g. PhNCO and the mixture stirred kept several hrs. gave 14 g. 2,6,3Cl2(MeO)C6H2CH:NO2CNHR (IV, R = Ph), m. 120-3° (decomposition). Similarly were prepared the following IV [R and m.p. (decomposition) given]: 4-ClC6H4, 130-1°; 1,2,3,4,5-Cl5C, 135°. 2,4,6-Cl3C6H2:NOH (45 g.) in 200 ml. Et2O treated dropwise at 20° with 24 g. PhNCO gave 57 g. 2,4,6-Cl3C6H2CH:NO2CNHPh, m. 154-6° (decomposition).
ACCESSION NUMBER: 1964:476345 CAPLUS
DOCUMENT NUMBER: 61:76345
ORIGINAL REFERENCE NO.: 61:13244b-g
TITLE: Chlorinated O-carbamoylbenzaldoximes
INVENTOR(S): Dickore, Karlfried; Sasse, Klaus; Eue, Ludwig; Heiss, Rudolf
PATENT ASSIGNEE(S): Farbenfabriken Bayer A.-G.
SOURCE: 6 pp.

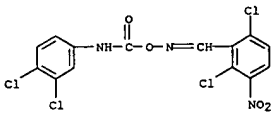
L31 ANSWER 82 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1174757		19640730	DE	19621222
BE 641600			BE	
FR 1379919			FR	
GB 995313			GB	
NL 302370			NL	

IT **92158-91-3**, Benzaldehyde, 2,6-dichloro-3-nitro-, O-[(p-chlorophenyl)carbamoyl]oxime **92167-56-1**, Benzaldehyde, 2,6-dichloro-3-nitro-, O-[(3,4-dichlorophenyl)carbamoyl]oxime **92428-75-6**, Benzaldehyde, 2,6-dichloro-3-nitro-, O-[(p-tolylsulfonyl)carbamoyl]oxime
(preparation of)
RN 92158-91-3 CAPLUS
CN Benzaldehyde, 2,6-dichloro-3-nitro-, O-[(p-chlorophenyl)carbamoyl]oxime (7CI) (CA INDEX NAME)

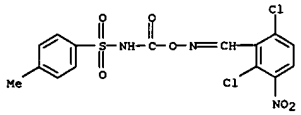


RN 92167-56-1 CAPLUS
CN Benzaldehyde, 2,6-dichloro-3-nitro-, O-[(3,4-dichlorophenyl)carbamoyl]oxime (7CI) (CA INDEX NAME)

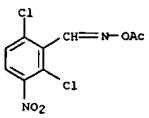


RN 92428-75-6 CAPLUS
CN Benzaldehyde, 2,6-dichloro-3-nitro-, O-[(p-tolylsulfonyl)carbamoyl]oxime (7CI) (CA INDEX NAME)

L31 ANSWER 82 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

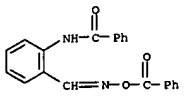


L31 ANSWER 83 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB The efficiency and phytotoxicity of various fungicides (zineb-S65, zineb P-10, maneb S-65, maneb P-7, maneb P-15, ferbam S-76, thiram S-80, and ziram S-80) against P. tabacina was studied in hot houses, sprout-beds, and in the field. Zineb at 0.3% concentration yielded very good results with no phytotoxic effect; 4-5 g./sq.m. of powder based on zineb (17.5-10%) yielded good results during field tests. Maneb (3-4 g./sq.m.), containing 7-17%, also yielded good results but a slight phytotoxic effect was observed. Maneb spray at 0.05-0.06% concentration was effective and medium phytotoxicity was of temporary character. Ferbam (0.5-0.47% concentration) provided effective protection without phytotoxicity. Thiram was effective at 0.4% concentration Ziram (0.2-0.4% concentration) failed to protect tobacco against P. tabacina.
ACCESSION NUMBER: 1964:19287 CAPLUS
DOCUMENT NUMBER: 60:19287
ORIGINAL REFERENCE NO.: 60:3430f-h
TITLE: Efficiency and phytotoxicity of some fungicides in protection of Dungansk tobacco from Peronospora tabacina
AUTHOR(S): Blagojevic, Milutin; Nadezdin, Milojka; Prpic, Zdenka
SOURCE: Agron. Glasnik (1963), 13(8), 559-67
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT **90418-11-4**, Benzaldehyde, 2,6-dichloro-3-nitro-, O-acetyloxime
(as fungicide)
RN 90418-11-4 CAPLUS
CN Benzaldehyde, 2,6-dichloro-3-nitro-, O-acetyloxime (7CI) (CA INDEX NAME)



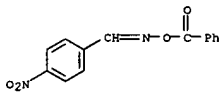
L31 ANSWER 84 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB Deoxygenation of quinazoline 3-oxide (I) to quinazoline (II) was effected by PCl3, PBr3, or catalytic reduction (Raney Ni). Such catalytic absorption of 1 mole equivalent H by 1.3 g. I in MeOH yielded 0.8 g. II, m. 48-9° (b. 240-3°), whereas absorption of 2 mole equivs. H by 0.75 g. I in MeOH yielded 0.3 g. 3,4-dihydroquinazoline, the structure of which (5 g.) in C6H6 was confirmed by oxidation with alkaline K3Fe(CN)6 to yield 2 g. II, b15-16 115-18°, m. 48°. However, I suffered ring fission with the anionoid reagents which caused simple substitution of the corresponding 1-oxide (III). Thus, 0.5 g. I and 0.23 g. KCN in H2O treated slowly with 0.5 g. BzCl gave an orange oil, purified by ether extraction and Al2O3 chromatography to yield 0.12 g. o-BzHNC6H4CH:NOBz, m. 147-8°, also formed, in confirmation of structure, from BzCl in C5H5N on o-H2NC6H4CH:NOH. I (0.5 g.) with p-MeC6H4SO2Cl in CHCl3 yielded 0.4 g. unidentified crystalline compound I (0.5 g.) heated 4 hrs. on a water bath with 6 cc. Ac2O, excess Ac2O removed in vacuo, the residue made alkaline with 15% K2CO3, extracted with C6H6, and the extract purified by Al2O3 chromatography yielded 0.08 g. o-CNC6H4CN, m. 109-10°, the infrared spectrum of which showed bands characteristic of CN and NC groups. I (0.5 g.) refluxed 1 hr. on a water bath with 10 cc. SO2Cl2 yielded 0.1 g. unidentified oil. Both unidentified products were probably also results of fission of the pyrimidine ring of I. Mechanisms for such reactions were outlined. Even 2N NaOH kept overnight at room temperature with 0.3 g. I opened the ring to yield 0.21 g. o-(OHCHN)C6H4CH:NOH, m. 154-5°. Reactions of the less reactive anionoid reagents with I afforded further contrasts to those with the 4-MeO derivative (IV) of III. Thus, 0.3 g. I allowed to stand overnight at room temperature with HCN-MeOH, 20% NaHSO3, or 80% N2H4.H2O gave, resp., 0.15 g. 4-NC derivative of II, m. 118-19° (identical with the oxidation product of 3,4-dihydro-4-quinazolinecarbonitrile), 0.25 g. 4-NaO3S derivative of II, m. above 360°, or 0.16 g. 4-H2NHN derivative (V) of II, m. 188-9° (decomposition). On the other hand, IV failed to react with HCN or NaHSO3 and with N2H4.H2O 0.3 g. IV yielded 0.2 g. 4-hydrazinoquinazoline 1-oxide, m. 167-8° (decomposition). The structure of V (0.35 g.) was confirmed by refluxing 3 hrs. on a water bath with BzH in MeOH to yield 0.2 g. 4-PhCH:NHN derivative of II, m. 171-2°. All these results indicated a greater nucleophilic activity of the 4-position in I as compared with the 2-position in III. Also, the 3-oxide group lessened the stability of the ring and led to its fission between the 2- and 3-positions.
ACCESSION NUMBER: 1962:38508 CAPLUS
DOCUMENT NUMBER: 56:38508
ORIGINAL REFERENCE NO.: 56:7320e-i,7321a
TITLE: Quinazoline 3-oxide
AUTHOR(S): Higashino, Takeo
CORPORATE SOURCE: Shizuoka Coll. Pharm.
SOURCE: Chemical & Pharmaceutical Bulletin (1961), 9, 635-41
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT **94963-92-5**, Benzanilide, 2'-formyl-, O-benzoyloxime
(preparation of)

L31 ANSWER 84 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 94963-92-5 CAPLUS
CN Benzanilide, 2'-formyl-, O-benzoyloxime (7CI) (CA INDEX NAME)

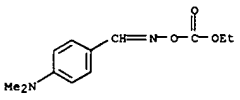


L31 ANSWER 85 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
AB H2NOBz (I), m. 8°, λ 230 mμ (ε 10,900) and 5.78 μ, was prepared from 15 ml. of a fresh 1:1 mixture of 4N H2NOH2Cl and 3.5N NaOH added with shaking to 20 millimoles p-O2NC6H4OBz (II), m. 145°, in 500 ml. 95% EtOH at 65° and allowed to stand 15 min. at room temperature, assays showing 100% p-O2NC6H4O- (by ε at 400 mμ) but only 15% hydroxamic acid (FeCl3 test); an addnl. 5 min. evaporation to 95 ml. at reduced pressure, addition of 95 ml. H2O, 2 extns. with 100 ml. Et2O, drying with Na2SO4, and evaporation produced 4.9 g. stable mixture, m. -15°, purified by washing a cold 1.5% solution in Et2O or CHCl3 with 0.2N aqueous Na2CO3, evaporating, and crystallizing at -78° from ether-petr. ether. From 157 mg. I in 5 ml. MeOH with 0.15 ml. Ac2O and 1.5 ml. M aqueous NaOAc at room temperature, evaporated to 0.5 ml. and crystallized from Et2O, was obtained 136 mg. AcNHOBz, m. 98-99°. I (42 mg.) with 45 mg. p-O2NC6H4CHO in 1.5 ml. HOAc gave an immediate precipitate from which, after standing 5 min., heating 10 min. on the steam bath and cooling, was isolated 59 mg. p-nitrobenzaldoxime benzoate, m. 192-2.5°. The same reactants in alc. without HOAc gave a mol. complex, m. 120°. It was attempted to prepare H2NOAc (III) similarly to I at 0° from H2NOH2Cl and 5 millimoles p-O2NC6H4OAc (IV), m. 78-9°; assays indicated p-O2NC6H4O-, 0.8 millimoles AcNHOH (V), and no Ac2NOH (VI); the distillate contained only alc. and 2.6 millimoles III, transformed into V and VI by attempted purification, or into 189 mg. BzNHOAc, m. 128-9°, with BzCl at room temperature Pure I after standing 2 hrs. (10 min.) at 30° (100°) decomposed into 45% (88%) BzNHOH and 11% (3%) Bz2NOH. In 1.6M H2NOH only BzNHOH was formed. I or III were completely destroyed by 0.01M NaOH in 5 min. at room temperature Other acylating agents for NH2OH were examined in neutral buffer solns. (in the presence of [CH2N(CH2CO2H)2]2 to prevent metal catalysis of N-acylation). Reagent and initial % hydroxamic acid (= N-acylation) are given: Ac2O 49, acetylimidazole 14, IV 25, VI 8, II 41, 2,4-(NO2)2 compound 63, BzCl 96.
ACCESSION NUMBER: 1959:77605 CAPLUS
DOCUMENT NUMBER: 53:77605
ORIGINAL REFERENCE NO.: 53:14030d-i
TITLE: Reaction of hydroxylamine with activated acyl groups. I. Formation of O-acylhydroxylamine
AUTHOR(S): Jencks, Wm. P.
CORPORATE SOURCE: Brandeis Univ., Waltham, MA
SOURCE: Journal of the American Chemical Society (1958), 80, 4581-4
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT **3848-35-9**, Benzaldehyde, p-nitro-, O-benzoyloxime (preparation of)
RN 3848-35-9 CAPLUS
CN Benzaldehyde, 4-nitro-, O-benzoyloxime (9CI) (CA INDEX NAME)

L31 ANSWER 85 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L31 ANSWER 86 OF 86 CAPLUS COPYRIGHT 2005 ACS on STN
GI For diagram(s), see printed CA Issue.
AB A kinetic study of the pyrolysis of acyl derivs. of the aldoximes, XC6H4CH:NOR → XC6H4CN + ROH, at various temps. in xylene and in the absence of solvents shows 1st-order kinetics, and the results of varying the substituent X indicate a decrease in the rate constant in the order o-MeO > p-Me2N > p-MeO > 3,4-CH2O2 > H > m-MeO > o-NO2 > m-NO2 = p-NO2. Variations in R produce a decrease in rate constant in the order Cl3CCO » Ph2NCO > EtOCO > p-NO2C6H4CO > Bz > p-MeOC6H4CO = CH2ClCO > Ac. If H bonding exists in the Ac derivs. of α-aldoximes, as suggested by Benger and B. (Part XXXIX, above), the pyrolysis can be represented as involving electron shifts without separation of charges (III). Electron release from XC6H4 favors the rupture of the N-O bond but hinders the rupture of the C-H bond, the effect from X = p-MeO to X = p-NO2 being less than in the hydrolysis of BzOEt. Electron withdrawal of R, while retarding the electron shift from the :O atom, favors it from the N-O bond, probably the determining factor in this reaction. Many pyrolyses are now regarded as involving a homolytic fission, but the absence of by-products in this reaction opposes this mechanism here. The rate consts. for o-NO2 compds. are appreciably higher than for the corresponding m- and p-NO2 isomers although the dissociation constant of o-O2NC6H4CO2H is 20 times that of the m- or p-isomer. These results suggest H bonding between the methine-H atom and an atom of the ortho-substituent, favoring rupture of the C-H bond (IV). Acyl derivs. prepared by known methods were: α-p-ON2C6H3CH: NOCOCH2Cl, m. 128°; α-p-MeOC6H3CH:NOCOCH2Cl, m. 72°; and α-m-NO2C6H3CH:NOBz, m. 175°. The following CO2Et derivs. were prepared (X in XC6H4CH:NOCO2Et and m.p., resp., given): m-NO2, 95°; p-NO2, 108°; o-NO2, 42°; o-MeO, 50°; H, 36-7°; p-MEO, 73°; and p-Me2N, 116°. α-m-MeOC6H3CH:NOOCOEt, m. 43° (from petr. ether), α-p-MeOC6H3CH:NOCOC6H4OMe-p, m. 149° (from C6H6), and p-MeOC6H3CH:NOOCOC6H4NO2-p, m. 153° (from C6H6), were also prepared
ACCESSION NUMBER: 1951:26920 CAPLUS
DOCUMENT NUMBER: 45:26920
ORIGINAL REFERENCE NO.: 45:4678g-i,4679a-e
TITLE: Isomerism of oximes. XLIII. Kinetics of the pyrolysis of acyl derivatives
AUTHOR(S): Ambrose, Douglas; Brady, O. L.
CORPORATE SOURCE: Univ. Coll., London
SOURCE: Journal of the Chemical Society, Abstracts (1950) 1243-9
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT **71063-92-8**, Benzaldehyde, p-dimethylamino-, α-O-ethoxycarbonyloxime (preparation of)
RN 71063-92-8 CAPLUS
CN Benzaldehyde, 4-(dimethylamino)-, O-(ethoxycarbonyl)oxime (9CI) (CA INDEX NAME)



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